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PART III

EVALUATION OF MOLECULAR WEIGHT FROM EQUILIBRIUM SEDIMENTATION

PART III. MOLECULAR WEIGHT DISTRIBUTIONS FROM EQUILIBRIUM SEDIMENTATION-DIFFUSION DATA VIA LINEAR PROGRAMMING

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FOREWORD

This report was prepared by the Polymer Branch of the Nonmetallic Materials Division. The work was initiated under Project No. 7342, "Fundamental Research on Macromolecular Materials and Lubrication Phenomena." Task No. 734203, "Fundamental Principles Determining the Behavior of Macromolecules," with Dr. M. T. Gehatia acting as task scientist. Coauthors are Mr. R. R. Jurick, ASD Computer Science Center (ASVC), and Dr. D. R. Wiff, Research Institute, University of Dayton. The work was administered under the direction of the Air Force Materials Laboratory, Directorate of Laboratories, Air Force Systems Command, Wright-Patterson Air Force Base, Ohio.

The report covers research conducted from September 1968 to August 1969. The manuscript was released by the authors in October 1969 for publication as a technical report.

This technical report has been reviewed and is approved.

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ABSTRACT

Within the past decade easy access to high speed digital computers has renewed interest in deriving molecular weight distributions from sedimentation-diffusion equilibrium data. One of the computational schemes which appears most promising is the Simplex Method of linear programming. The purpose of this work was to investigate the advantages and limitations of this approach.

It was found that, even though inferring a molecular weight distribution from sedimentation-diffusion equilibrium data is mathematically an ill-posed problem, the method of linear programming yields qualitatively a good molecular weight distribution. Also, the method proved satisfactory for the case when sedimentation equilibrium data was acquired from only a single angular velocity.

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SECTION I

INTRODUCTION

The relationship describing sedimentation-diffusion equilibrium of an ideal polydisperse solution in an ultracentrifuge can be given by a Fredholm integral equation of the first kind (Reference 1). Since no rigorous solution of this integral is known, there have been many attempts to solve it by approximation (References 2, 3). These efforts mainly involved use of Fourier transforms or Laplace transforms by assuming an approximate functional expression for the experimental concentration gradient along the ultracentrifugal cell, or by expanding the molecular weight distribution (MWD) into a polynomial of assumed functions.

The main weakness has been that some parts of the calculated distribution would be negative. Physically, of course, we know that the MWD for any molecular weight must always be positive or zero. Recently Lee (Reference 4) carried out an investigation of the Fredholm integral equation and found that mathematically it is an "ill-posed" problem. In trying to infer a MWD from experimental measurements of concentration gradients small errors can lead to an unacceptable MWD. Therefore, we compromised in trying to determine only an "overall" shape of the MWD without being specific to individual points, i.e., we allowed certain fluctuations of the curve to be present and ignored fine structure.

To generalize a theoretical analysis, let us accept that the MWD can be slightly negative for some molecular weight values. Since we chose to ignore the point-by-point functional form of the MWD, the next logical step would be to subdivide the MWD into narrow (not infinitesimal) but finite molecular weight strips. This would result in approximations of MWD by rectangles of finite width and would lead naturally to the use of matrices. This has been done (Reference 5) but unfortunately the matrices are "ill-conditioned" or nearly singular.

Scholte (Reference 6 and 7) in 1968, still using matrices, applied the scheme of linear programming to infer a MWD from experimental measurements of concentration gradients at various angular velocities. The main

advantage to this approach is that values of the MWD are forced to be greater than or equal to zero and "slack variables" are introduced to account for experimental error. Scholte evaluated the MWD at ten molecular weights, then shifted to ten other molecular weights in a prescribed manner, continuing until, finally, there were four such sets. Since each set represented an individual solution, one quarter of the sum of the four sets also represented a solution. By doing this, Scholte obtained good agreement between his assumed and calculated molecular weight distributions.

There are, however, three reasons why Scholte's scheme cannot be blindly applied to other systems. These are: (1) Scholte dealt with a molecular weight range of 5×10^4 to 10^6; by comparison, in many cases of synthetic polymers the range is much narrower, e.g., 0 to 10^5. (2) Scholte used five or more angular velocities, each requiring several days for equilibrium. There are, however, cases when equilibrium at each velocity requires a much longer time (Reference 8). Therefore, it is important to have a scheme which would produce a MWD from data taken at one velocity. (3) Since our interest was in a different molecular weight range and we were using experimental data from only one angular velocity, the effects of experimental error on the calculated MWD had to be investigated.

A computer program using Scholte's ideas was independently coded and a different linear programming (LP) solving routine was employed. The new program reliability was verified by reproducing Scholte's published results. Then application of the new program to new specific needs stated above were investigated. A brief description of linear programming theory follows.

SECTION II

THEORY

In the brief discussion which follows, all theorems and definitions are given without proof or examples. All material on linear programming was taken from other works (References 9, 10, and 11).

Definition 1. A simplex is an n-dimensional convex polyhedron having exactly n+1 vertices. The boundary of the simplex contains simplical faces of dimension i where $i < n$. The number of such faces of dimension i is $\binom{n+1}{i+1}$ where $\binom{n}{m} = n!/m!(n-m)!$. A simplex in zero dimension is a point, in 1-dimension a line, in 2-dimension a triangle, in 3-dimension a tetrahedron, etc. The equation of a simplex with unit intercept is $X_i \geq 0$ and $\sum_i X_i = 1$.

Definition 2. A subset C of E_n (n-dimensional Euclidean Space) is a convex set if and only if for all pairs of points $\underline{V}_1$ and $\underline{V}_2$ in C any convex combination

$$\underline{V} = \beta_1 V_1 + \beta_2 V_2 \qquad (1)$$

is also in C, where β_i are scalars, $\beta_i \geq 0$, and $\sum_i \beta_i = 1$.

Definition 3. A point $\underline{V}$ in a convex set C is called an extreme point if $\underline{V}$ cannot be expressed as a convex combination of any other two distinct points in C. That is, if we denote the convex set of solutions to the linear programming problem by K and if K is a convex polygon, then K is the convex hull of the extreme points of K. Therefore, every feasible solution in K can be represented as a convex combination of the extreme feasible solutions in K.

Theorem 1. The set of all feasible solutions to the linear programming problem is a convex set.

In general, the linear programming problem can be described as follows: Given is a convex set defined by a set of linear constraints in E_n. From all the points belonging to the convex set, we wish to determine a subset of points (which will contain either one or many points) for which a linear objective function is optimized.

Usually we are confronted with a set of simultaneous equations

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + a_{13}x_3 + \cdots + a_{1m}x_m &= b_1 \\ \vdots \qquad\qquad & \qquad\qquad \vdots \\ a_{n1}x_1 + a_{n2}x_2 + a_{n3}x_3 + \cdots + a_{nm}x_m &= b_n \end{aligned} \tag{2}$$

where $n > m$. For simplicity let m equal n; let A be the matrix, $\left\{a_{ij}\right\}$, (i = 1, 2, 3, --- m and j = 1, 2, 3---m); $\underline{X}$ the vector $\left[X_j\right]$, j = 1, 2, 3---m and $\underline{b}$ the vector $\left\{b_i\right\}$, i = 1, 2, 3---, m. Then Equation 2 can be written in the form

$$A\underline{x} = \underline{b} \tag{3}$$

Since A is a square matrix and assumed nonsingular, the solution vector is expressed as

$$\underline{x} = A^{-1}\,\underline{b} \tag{4}$$

A simple computational scheme is the complete elimination method of Jordan and Gauss which has a finite number of steps or iterations. In just m iterations the procedure multiplies the system (Equation 2) by A^{-1} to obtain Equation 4. This is the standard matrix problem which is assumed familiar to the reader.

Now, in linear programming the problem is reversed. Instead of having an "over-determined" system as indicated by Equation 2, we have an "under-determined" system (i. e., $n < m$) subject to other constraints. That is, we wish to find a vector $\left\{x_i\right\}$, i = 1, 2, 3, ---m which minimizes the linear form (i. e., the objective function)

$$C_1x_1 + C_2x_2 + C_3x_3 + - - - + C_mx_m \tag{5}$$

subject to linear constraints

$$x_j \geq o, \quad j = 1, 2, 3, ---, m \tag{6}$$

and the set of equations given by Equation 2 but with $n < m$.

For large n and m it would be an impossible task to evaluate all possible solutions and select one that minimizes the objective function. A computational

scheme is desired which converges to a minimum solution. The Simplex Method, devised by Dantzig (Reference 11) is such a scheme. In Reference 11 the equation $\sum X_i$ is used as a constraint. The procedure finds an extreme point and determines whether it is the minimum. If it is not, the procedure finds a neighboring extreme point whose corresponding value of the objective function is less than or equal to the preceding value. In a finite number of such steps (usually between n and 2n), a minimizing feasible solution is found. The Simplex Method makes it possible to discover whether the problem has any finite minimizing solutions or no feasible solutions at all.

Consideration is now given to how this can be related to the problem at hand, namely, molecular weight determination via sedimentation-diffusion equilibrium. The equation describing sedimentation-diffusion equilibrium for a heterogeneous system is given (from Reference 1) by

$$-\frac{1}{C^{o}}\frac{dC}{d\xi} = \int_{0}^{\infty} \frac{\lambda^2 M^2 e^{-\lambda M} F(M)}{1 - e^{-\lambda M}}\, dM \qquad (7)$$

where,

$$\int_{0}^{\infty} F(M)\, dM = 1 \qquad (8)$$

In the above equations C° is the concentration of the original solution, C is the equilibrium concentration at radial distance r, M is the molecular weight, F(M) is the frequency function of molecular weight, $\xi = (r_b^2 - r^2)/(r_b^2 - r_m^2)$ with r_m the radial distance from the center of rotation to the meniscus, and r_b the radial distance from the center of rotation to the bottom of the cell. Also, $\lambda = (1-v\rho)\,\omega^2 (r_b^2 - r_m^2)/2RT$, where v is the partial specific volume of the dissolved substance, ρ is the density of the solution, ω is the angular velocity in radian per second, R is the gas constant, and T the absolute temperature.

Rewriting Equations 7 and 8 for the discrete case (Dirac δ -functions) one obtains

$$U(\lambda_i \xi_n) = \sum_{m} \frac{\lambda_i^2 M_m^2 e^{-\lambda_i M_m \xi_n}}{1 - e^{-\lambda_i M_m}} f_m \qquad (9)$$

and,

$$\sum_m f_m = 1 \tag{10}$$

where

$$U(\lambda_i, \xi_n) = -\frac{1}{C^\circ}\left(\frac{dC}{d\xi_n}\right)_{\lambda_i} \quad \text{and} \quad f_m$$

is the weight fraction of molecules of a given molecular weight M_m in the original sample. Recall that the $U(\lambda_i, \xi_n)$ and ξ_n are the experimentally measured quantities with λ_i being the product of a constant (determined from auxiliary measurements) and the square of the angular speed of the rotor.

For convenience of notation let

$$K_{\ell n} = \frac{\lambda_i^2 M_m^2 e^{-\lambda_i M_m \xi_n}}{1 - e^{-\lambda_i M_m}} \tag{11}$$

and

$$U_\ell = U(\lambda_i, \xi_n) \tag{12}$$

where for each i, n = 1, 2, ---N; i = 1, 2, ---, I; m = 1, 2, ---M; and ℓ = 1, 2, ---, L with L = IN and L > M.

Thus Equation 9 becomes

$$U_\ell = \sum_m K_{\ell m} f_m \tag{13}$$

Since the quantities of U_ℓ are experimentally measured, they will in all probability be greater than or less than their true precise value (i.e., there exists experimental error). Although this physical fact is accepted, experimentally Equation 13 does not hold true. This is especially apparent when we investigate the matrix $\{K_{\ell m}\}$ and find it ill-conditioned. In essence, the matrix $\{K_{\ell m}\}^{-1}$ acts as an "amplifier" for any error which might exist in the set $\{U_\ell\}$.

If we grant that an error in U_ℓ exists, Equation 13 becomes

$$U_\ell = \sum_m K_{\ell m} f_m + \epsilon_\ell \tag{14}$$

where ϵ_ℓ is the experimental error in U_ℓ. Since the application of linear programming necessitates that all x_i (see Equation 1) are positive or zero, we must account for error's being positive or negative. It is the inclusion of error that now enables us to go from an "over determined" system to an "under determined" system. The linear programming procedure is now applicable. In particular, you will recall that a modified Simplex Method can be used.

Recapitulating, we now obtain the formulation of the linear programming scheme as used to determine the MWD from sedimentation-diffusion equilibrium. We wish to find the set $\{f_m\}$, $m = 1, 2, \cdots Q$, which minimizes the linear form (i.e., the objective function)

$$\sum_{\ell=1}^{L} (\delta_\ell + \beta_\ell) \tag{15}$$

subject to the linear constraints

$$\left.\begin{aligned} f_m &\geq 0, \quad m = 1, 2, 3, \cdots Q \\ \delta_\ell &\geq 0 \\ \beta_\ell &\geq 0 \end{aligned}\right\}, \ell = 1, 2, 3, \cdots L \tag{16}$$

and

$$\begin{aligned} K_{11}f_1 + K_{12}f_2 + \cdots + K_{1Q}f_Q + \delta_1 - \beta_1 + 0 + 0 + \cdots + 0 + 0 &= U_1 \\ K_{21}f_1 + K_{22}f_2 + \cdots + K_{2Q}f_Q + 0 + 0 + \delta_2 - \beta_2 + \cdots + 0 + 0 &= U_2 \\ \vdots \\ K_{L1}f_1 + K_{L2}f_2 + \cdots + K_{LQ}f_Q + 0 + 0 + 0 + 0 + \cdots + \delta_L - \beta_L &= U_L \end{aligned} \tag{17}$$

where $L > Q$**. Let the set $\{x_i\}$, $i = 1, 2, 3, \ldots, Q + 2L$ be composed of f_m values for $i = 1, 2, 3, \cdots Q$, and alternately δ_ℓ and β_ℓ for $i = Q + 1, Q + 2, \cdots$, $Q + 2L$; where all $X_i \geq 0$. Also let the $L \times (Q + 2L)$ matrix P be represented by

**This is not an absolutely necessary condition. When one velocity was used the situation arose where $L < Q$.

$$P = \begin{pmatrix} K_{11} & K_{12} & \cdots & K_{1Q} & 1 & -1 & 0 & 0 & \cdots & 0 & 0 \\ K_{21} & K_{22} & \cdots & K_{2Q} & 0 & 0 & 1 & -1 & \cdots & 0 & 0 \\ \vdots & & \ddots & \vdots & & \vdots & & & \ddots & \vdots & \\ K_{L1} & K_{L2} & \cdots & K_{LQ} & 0 & 0 & 0 & 0 & \cdots & 1 & -1 \end{pmatrix} \qquad (18)$$

Then, in matrix notation the problem is formulated by

$$P\underline{X} = \underline{U} \qquad (19)$$

The next section will describe the application of this method.

SECTION III

VARIABLE FACTORS IN COMPUTATION AND THEIR INFLUENCE ON RESULTING MWD

A. FORMULATION OF COMPUTER PROBLEM

The objective of this section is to present the results which three variable factors investigated have on a MWD. Since the actual programming involved a slight modification of Equation 9, a listing and discussion of the variable factors investigated will be preceded by a discussion of the actual equation programmed.

The programmed equation is given by

$$U(\lambda_k, \xi_i) = \sum_n \frac{\lambda_k^2 M_n^2 e^{-\lambda_k M_n \xi_i} F(M_n) \Delta M_n}{1 - e^{-\lambda_k M_n}} \qquad (20)$$

Here all quantities have the same meaning as in Equation 7 and 9. However, we must remember that, since λ is proportional to the square of the angular velocity, the index k indicates the various velocities at which equilibrium was achieved. For each velocity there exists a set of ξ-values, i.e., for each λ_k there is a corresponding set $\{\xi_i\}$. If there are data from five velocities and for each velocity there corresponds five ξ - values, this would imply twenty-five U -values. It is imperative that the molecular weight range being investigated incorporate all molecular weights present in the solution sample being centrifugated. Since Equation 9 and 20 deal with discrete molecular weights, some procedure must be employed to span the entire molecular weight range (MWR). Following the idea of Scholte (References 6 and 7), a multiplicative factor (g-factor) has been introduced. Therefore, starting with the first molecular weight M_1, the other molecular weights in a given sampled set could be generated. Knowing, a priori, the MWR we can now calculate the g-factor and the number (N_Q) of molecular weights needed to span the MWR. (The g-factor is later used as a variable parameter related to the error in the experimental concentration gradients. However, the value of g must be at least large enough to ensure the actual MWR present in a given experiment

is spanned. A convenient technique for finding the MWR is given in Reference 8). The molecular weights sampled will be

$$M_n = M_1 g^{n-1} \tag{21}$$

where $n = 1, 2, 3, ---, N_Q$. This enables one to divide the MWR into non-overlapping subranges. Each subrange span is denoted by

$$\Delta M_n = M_n - M_{n-1} \tag{22}$$

where M_o is assumed zero. By employing the averaging technique of Scholte (Reference 7), after solving Equation 20 for one set of molecular weights, a new set of molecular weights is selected in a prescribed manner. The new set is shifted relative to the previous set by a multiplicative factor $g^{1/N}$, where N is the number of desired molecular weight sets. That is, if the number of the set is labeled by the index n and the molecular weights within a set by j, then

$$M_{j,n} = M_{1n} g^{j-1} \tag{23}$$

and

$$\Delta M_{jn} = (g^{1/2} - g^{-1/2}) M_{jn} \tag{24}$$

where $j = 1, 2, 3, ---, NQ$; $n = 1, 2, 3, ---, N$; and $M_{o,n} = O$.

The concentration of molecular weights in a given subrange is simply the weight fraction (f_m) multiplied by the initial solution concentration ($C°_m = C°f_m$). When Scholte (Reference 7) presents his final results they are in the form MF(M) versus M. In this work a modified system F(M) versus M has been calculated (Equation 20), since one usually has less qualitative feeling for MF(M) than for F(M).

Now, it is possible to list the variable parameters investigated in this work. They are as follows:

1. The effect that varying the g-factor (i.e., the span of the molecular weight subrange) has on the resulting MWD; and also the effect when the number of sets of molecular weights sampled was varied.

2. How the resulting MWD is affected by varying the number of elements in the sets $\{\xi_i\}$ and $\{\lambda_k\}$.

3. Whether the introduction of error into idealized U-values affects the resulting MWD. This includes normal random error and weighted random error.

The results of each will be discussed successively in the following section.

B. DISTRIBUTIONS STUDIED

The g-factor is related to the experimental error in the U-values (Reference 7). Figures 1 through 4 show the effect of varying the g-factor and the number of sets of molecular weights. In each case the solid-line curve is the assumed distribution from which U-values were calculated. For all curves, seven velocities were used and with each velocity five ξ -values. The squared angular velocities were 4.1693×10^5, 5.8370×10^5, 8.1718×10^5, 11.4406×10^5, 16.0168×10^5, 22.4235×10^5, and 31.3929×10^5 rad^2/sec^2 with $\xi = 0$, 1/4, 12, 3/4, and 1 for each case. Therefore, thirty-five U-values were used for these calculations.

As previously mentioned, we must always be sure that the MWR is wide enough to incorporate all molecular weights present in the sample. To study the effect of range size on the MWD, all parameters in Figure 4 were held constant except the value for MWR, which was brought closer to the MWR of the assumed distribution. As shown in Figure 5, structure begins to appear when the highest molecular weight sampled was not far beyond the actual highest molecular weight present. Figure 5 represents a calculation involving twenty molecular weight sets. When the number of molecular weight sets was decreased from twenty to ten (Figure 6) then five (Figure 7), there was no appreciable change except that, naturally, the calculated points were spaced farther apart.

What would be the effect if the number of ξ -values associated with each velocity was increased? As previously mentioned, five ξ -values have been used per velocity for Figures 1 through 7. Figure 8 shows the results with all

parameters of Figure 6 held constant except that, now, nine ξ-values were used. The nine ξ-values were so chosen that $\xi = 0$ to 1 with $\Delta\xi = 1/8$. From the study of this assumed distribution it appears that using five ξ-values, sampling twenty sets of molecular weights, and using a g-factor ≈ 2.0 seemed to have produced the optimum desired results, i.e., the calculated MWD agreeing best with the assumed MWD. If the g-factor became too small the result was noise, that is, the accuracy of the U-values did not warrant such precision, or the matrix in the LP solver routine became singular.

At this stage a normal Gaussian distribution with a MWR of 0 to 120,000 was investigated. Once again the g-factor was varied. The lowest g-value used was 1.15 and the highest 4.0. The former resulted in an erratic MWD and the latter resulted in a curve which went exponentially to zero at high molecular weights. The best g-value for this specific case was $g = 1.8$. In general, a satisfactory technique was to start with a low value of g. Then as the value of g was increased the erratic behavior of the MWD disappeared. At the g-value where the erratic results seemed to disappear, that value was established as the appropriate one. Then the maximum reliable "fine structure" for a given set of experimental U-values was attained.

Using this assumed normal distribution (its functional form) the MWR was shifted to investigate the reliability of the method for various molecular weight ranges. One range tried was from 0 to 12,000 and another from 10^5 to 10^6. In each case the results were satisfactory, considering that in all cases g was kept constant ($g = 1.8$).

As previously mentioned, the U-values used resulted from seven assumed velocities ranging from about 6,000 to 50,000 RPM. It would be advantageous if the experimental U's were obtained from an equilibrium sedimentation-diffusion experiment at only one angular velocity. To check this, the normal Gaussian distribution, MWR from 0 to 120,000, was approximated (holding all other variables constant) by deleting all U-values associated with various angular velocities. All combinations of the velocities were tried. By using only the lowest angular velocity (6,166 RPM), the computer program produced a MWD which "fit" the assumed MWD as well as the case where all seven angular velocities were used. In fact, all single velocity cases resulted in

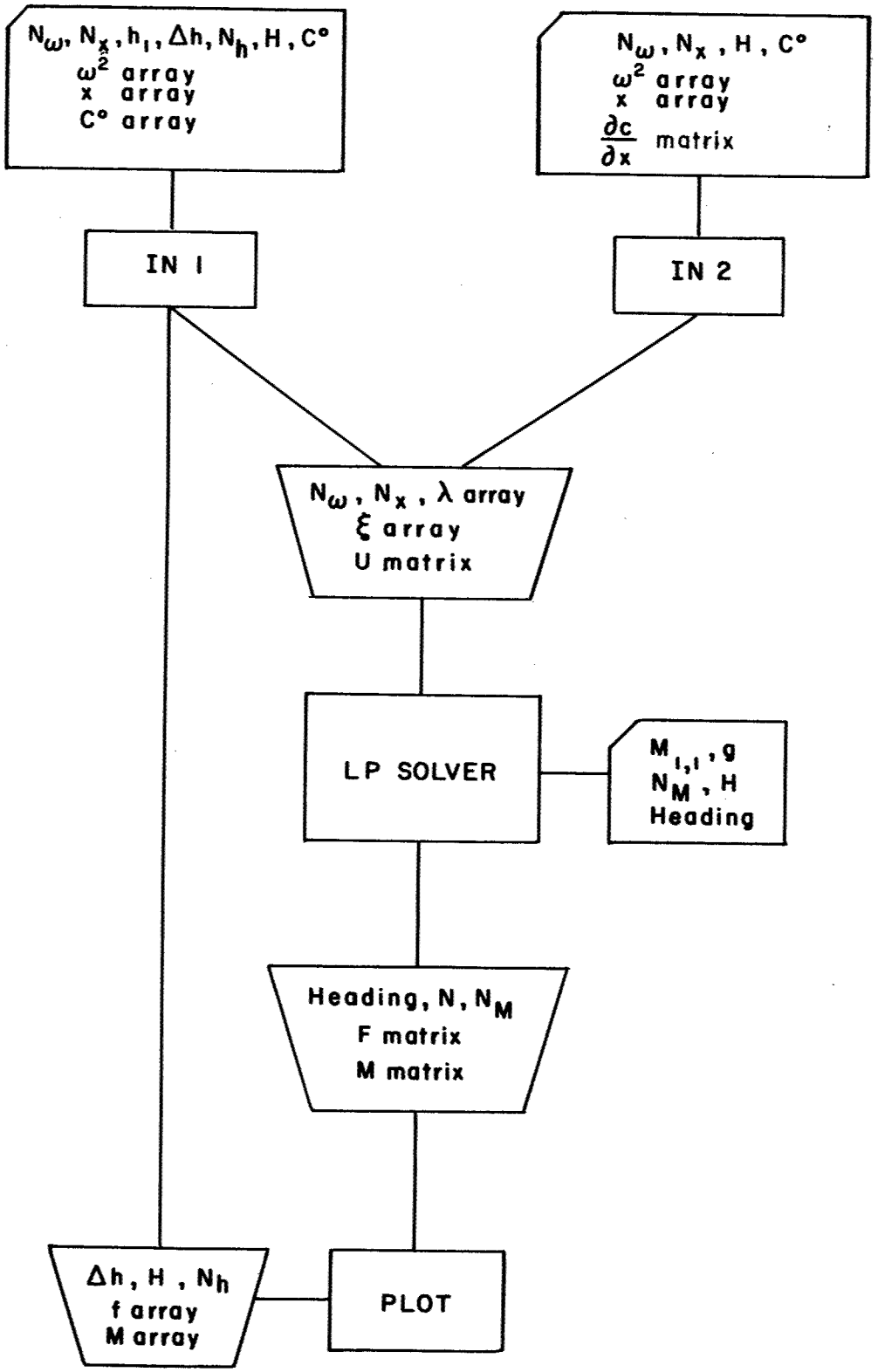
a reasonable MWD. Therefore, we would conclude that an acceptable MWD could be obtained from an equilibrium sedimentation-diffusion experiment at one angular velocity, at least with a MWR of 0 to 120,000.

The third area of investigation involved use of the normal Gaussian MWD ($0 < M < 120,000$) U-values from one angular velocity (6,166 RPM) and at $\xi = 0$, 1/4, 1/2, 3/4, and 1 to find the effect that error in the U-values would have on the calculated MWD. Error (1, 2, 5, 10, and 20%, respectively) was introduced by aid of a random error generator. For each magnitude of error, five calculations were employed to vitiate any wrong conclusions that one error distribution might have on the final MWD. For each case (1 to 20%) when the error was normally distributed (dotted line Figure 9) the calculated MWD agreed with the assumed MWD. Naturally the 1% error case gave the best "fit" to the assumed MWD, but even for the 20% error case the calculated MWD was not unacceptable. When the error introduced in the U-values was such as to be weighted (dashed curves Figure 9), the calculated MWD was entirely different from the expected normal MWD. This phenomenon substantiates the findings of Lee (Reference 5) and Tikhonov and Glasko (Reference 12).

SECTION IV

DESCRIPTION OF COMPUTER PROGRAM

FLOW DIAGRAM



DESCRIPTION OF VARIABLES

a_{i_j} - entry in matrix for LP problem

b - largest x value

b_i - right-hand side of LP problem

$C°$ - initial concentration of solution

$C°_m$ - initial concentration of solution whose molecular weight is $\frac{h_n}{H}$

f_n - weight fraction of molecular weight M_n

$F_{j,n}$ - results of LP solution, frequency list for mol. wt. of $M_{j,n}$

g - M multiplier

h_n - input test array which is a function of molecular weight (References 5 and 8)

$H = \frac{2RT}{1-v\rho}$

m - smallest x value

M_n - molecular weight array associated with input test array

$M_{j,n}$ - molecular weight matrix of values used in LP solution

N - number of LP sets to try

N_h - number of input h values

N - number of M values to use for use LP solution

N_ω - number of input ω^2 values

N_x - number of input x values

$U_{k,\ell} = -\frac{1}{C°}\frac{dc}{d\xi}$

x_ℓ - array of distances squared from center of rotation

λk - function of $\omega^2 k$

Δh - constant difference between values of h_n array

$\Delta M_{j,n}$ - difference between successive j values of $M_{j,n}$ matrix

ξ_{ℓ_2} - function of x_ℓ

ω^2 - square of the angular velocity

IN 1 ROUTINE

Input: N_ω N_x, h_1, Δh, N_n, H, C°, ω_k^2 array, where $k = 1, ---, N_\omega$

x_j array, where $\ell = 1, ---, N_x$

$C°_n$ array, where $n = 1, ---, N_h$

1. $h_{n+1} = h_n + \Delta h$ for $n = 1, ---, (N_h - 1)$

2. $m = x_1$

   $b = x_{N_x}$

   $\lambda k = (b-m) \cdot H \cdot \omega_k^2$ for $k = 1, ---, N_\omega$

3. $\xi_\ell = \frac{b-x_1}{b-m}$ for $\ell = 1, ---, N_x$

4. $M_n = \frac{h_n}{H}$ for $n = 1, ---, N_h$

   $f_n = \frac{C°_n}{C°}$

5. $U_{k,\ell} = \sum_{n=1}^{N_h} \frac{(\lambda_k M_n)^2 \, e^{-\lambda_k M_n \xi_\ell}}{1 - e^{-\lambda_k M_n}} f_n$

   for $k = 1, ---, N_\omega$ and $\ell = 1, ---, N_x$

6. Write out ω^2 array, ξ array, and U matrix

7. Call LP SOLVER

IN 2 ROUTINE

Input: N_ω, N_x, H, C°, ω_k^2 array where $k = 1, ---, N_\omega$

x_ℓ array where $\ell = 1, ---, N_x$

$(\frac{dC}{dx})_{k\ell}$ matrix where $k - 1, ---, N_\omega$ and $\ell = 1, ---, N_x$

1. $m = x_1$

   $b = x_{n_x}$

2. $\lambda k = (b-m)\ H\ \omega_k^2$ for $k = 1, ---, N_\omega$

3. $\xi_\ell = \frac{b-x_\ell}{b-m}$ for $\ell = 1, ---, N_x$

4. $U_{k,\ell} = \frac{b-m}{C°}\ (\frac{dc}{dx})_{k,\ell}$ for $k = 1, ---, N_\omega$ and $\ell = 1, ---, N_x$

5. Write out ω^2 array, ξ array, and U matrix

6. Call LP SOLVER

LP SOLVER

1. Input from IN 1: N_ω, N_x, λ array, ξ array, and U matrix

2. Input from cards: $M_{1,1}$, g, N_M, N, HEADING

3. Write out input from cards

4. N_{row} N_ω: N_x

   $N_{col} = N_M + 2 N_{row}$

   $n = 1$

5. Calculate the following matrix entries

   $a_{i_j} = 1$ for $i = 1, ---, N_{row}$ and $j = N_M + 1, N_{col-1}, 2$

   $a_{i_j} = 1$ for $i = 1, ---, N_{row}$ and $j = N_M + 1, N_{col}, 2$

   $$a_{i_j} = \frac{(\lambda_k M_{j,n})^2 \; e^{-\lambda_k M_{j,n}} \xi_\ell}{1 - e^{-\lambda_k M_{j,n}}} \Delta M_{j,n}$$

   for $i = 1, ---, N_{row}$ and $j = 1, ---, N_M$

   where $k = \left[\frac{i-1}{N_x}\right] + 1$

   $$\ell = i - (k-1) \cdot N_x$$

   $$M_{j,n} = M_{1,n} \cdot g^{j-1}$$

   and

   $$\Delta M_{j,n} = (g^{1/2} - g^{-1/2}) M_{j,n}$$

6. Calculate the following right-hand sides $b_i = U_{k,\ell}$ where i, k, and ℓ are defined as in step 5.

7. Calculate the following objective coeffcients

   $C_j = O$ for $j = 1, ---, N_M$

   $C_j = 1$ for $j = N_M + 1, ---, N_{col}$

LP SOLVER

8. Write out the determinants of:

   $\left[a_{i_j} \right]$ for $i = 1, ---, N_M$ and $j = 1, ---, N_M$

   $\left[a_{i_j} \right]$ for $i = N_M + 1, ---, 2 \cdot N_M$

   $\left[a_{i_j} \right]$ for all sets of N_M rows less than N_{row}

9. Write out matrix $\left[a_{i_j} \right]$ for $i = 1, ---, N_{row}$ and $j = 1, ---, N_M$ in exponent form.

10. Call LP solver and store solutions in $F_{j,n}$ array.

11. Write out input RHS
    computer RHS using solution
    difference of RHS'S
    absolute value of relative differences of RHS
    average absolute relative difference

12. $n \leftarrow n + 1$

    $M_{1,n} \leftarrow (M_{1,n-1})g^{1/N}$

13. Return to step 5 until n exceeds N

14. Write out $F_{j,n}$ matrix

15. Call PLOT routine

PLOT ROUTINE

1. Input from LP SOLVER: HEADING, N, N_m, F, and M matrices
2. Input from IN 1 (if used): Δh, H, N_n f, and M arrays
3. $\Delta M = \frac{\Delta h}{H}$
4. Write out heading
5. Label vertical axis F(M)
6. Label horizontal axis M
7. Plot $\frac{f_n}{\Delta M}$ versus M_n for n = 1, ---N_h
8. Plot $F_{j,n}$ versus $M_{j,n}$ for n = 1, ---N and j = 1, ---, N_M
9. STOP

SECTION V

CONCLUSION

To date, the linear programming method seems to be one of the most promising schemes for obtaining the molecular weight distribution from sedimentation-diffusion equilibrium data. There are five main features of this investigation which are worthy of mention.

1. The linear programming method has been found to give acceptable results for the case of experimental data obtained at one angular velocity.

2. It was found that if a normal random error of the experimental gradient curve was about 20% the linear programming method produced a MWD with satisfactory precision. However, if the experimental error was weighted, i.e., the concentration gradient curve was distorted from the true curve, a 1 or 2% error led to an absurd molecular weight distribution. This agrees with the findings of Lee (Reference 5), Tikhonov and Glasko (Reference 12), and Tikhonov (References 13 and 14).

3. This investigation did not involve any modification of the LP solver routine. The LP solver limitations were manifested by spurious points sometimes appearing in the determined molecular weight distribution. In general, the linear programming method presents only an overall molecular weight structure. Therefore, when twenty sets of molecular weights were sampled, it was obvious when one point was completely illogical.

4. A great improvement was achieved by solving for F(M) directly (Equation 20), rather than via f_m (Equation 9). In the former case the matrix presented to the LP solver routine was not so ill-conditioned (Tables I and II).

5. The following test was made after each call of the LP solver routine. By having the calculated MWD, the computer program could calculate new U-values (U_{calc}). The difference between U_{exp} and U_{calc} was then printed. Also, the absolute relative differences, the averaged absolute relative error for one set of molecular weights, and the averaged absolute relative error averaged over all molecular weight sets were printed. In general, a good "fit" between the assumed MWD and the derived MWD showed low values for

all the above error analyses; however, the converse was not always found to hold true. At present much effort is being focused on determination of a procedure for obtaining a one-to-one correspondence between the error analysis criteria and the "fit" of the derived MWD.

TABLE I

EXPONENTS OF ELEMENTS IN THE MATRIX PRESENTED TO LP SOLVER ROUTINE USING EQUATION 9 *

-2	-1	-1	-1	0	0	0	0	0	0
-2	-1	-1	-1	0	0	0	0	0	0
-2	-1	-1	-1	0	0	0	0	0	0
-2	-1	-1	-1	0	0	0	0	0	0
-2	-1	-1	-1	0	0	0	0	0	1
-1	-1	0	0	0	0	0	0	-2	-5
-1	-1	0	0	0	0	0	0	-1	-3
-1	-1	0	0	0	0	0	0	0	-1
-1	-1	0	0	0	0	0	0	0	0
-1	-1	0	0	0	0	0	1	1	2

* Value of determinant = -0.3932972 E-31

TABLE II

EXPONENTS OF ELEMENTS IN THE MATRIX PRESENTED TO LP SOLVER ROUTINE USING EQUATION 20*

1	1	2	3	3	4	4	5	5	5
1	1	2	3	3	4	4	5	5	5
1	1	2	3	3	4	4	5	6	6
1	1	2	3	3	4	5	5	6	6
1	1	2	3	3	4	5	5	6	7
1	2	3	3	4	4	4	4	3	0
1	2	3	3	4	4	5	5	4	2
1	2	3	3	4	4	5	5	5	4
1	2	3	3	4	5	5	6	6	6
1	2	3	3	4	5	5	6	7	8

* Value of determinant = -0.1500715 E 17

APPENDIX

LISTING OF COMPUTER PROGRAM

```
$IBFTC EXEC.   DECK                                                    EXEC.001
C                                                                      EXEC.002
C      MAIN PROGRAM EXECUTIVE CONTROL                                  EXEC.003
C         INITIALIZE PLOTTING ROUTINES                                 EXEC.004
C         INITIALIZE PLOT COUNT                                        EXEC.005
C         DETERMINE SEQUENCE OF SUBROUTINES CALLED                     EXEC.006
C         TERMINATE PLOTTING BEFORE EXITING                            EXEC.007
C         WRITE HEADING AND PLOT COUNT                                 EXEC.008
C                                                                      EXEC.009
      COMMON /PLTR/ PDATA(438), IPLTS, HEAD(12)                        EXEC.010
      COMMON  /PRTCTL/  WRITE                                          EXEC.011
C                                                                      EXEC.012
      LOGICAL WRITE                                                    EXEC.013
C                                                                      EXEC.014
      IPLTS = 0                                                        EXEC.015
      CALL PLOTS ( PDATA, 438 )                                        EXEC.016
    1 READ (5,500) HEAD                                                EXEC.017
      WRITE (6,600) HEAD                                               EXEC.018
      CALL IN1 ( $900 )                                                EXEC.019
      IF ( WRITE )  WRITE (6,600) HEAD                                 EXEC.020
      CALL LPS ( $900 )                                                EXEC.021
      CALL PLOTR                                                       EXEC.022
      GO TO 1                                                          EXEC.023
  900 WRITE (6,601) IPLTS                                              EXEC.024
      CALL PLOTE                                                       EXEC.025
      STOP                                                             EXEC.026
  500 FORMAT ( 12A6 )                                                  EXEC.027
  600 FORMAT ( 1H1, 12A6  / ( 1X, 12A6 ) )                             EXEC.028
  601 FORMAT ( 1H0, I2, 17H PLOT(S) COMPLETE )                         EXEC.029
      END                                                              EXEC.030
```

```
$IBFTC BIN1.   DECK                                                    BIN1.001
C                                                                      BIN1.002
C      BLOCK DATA SUBPROGRAM TO SUPPLY INPUT DATA WHEN INP1. IS BY-PASSEDBIN1.003
C                                                                      BIN1.004
       BLOCK DATA                                                      BIN1.005
C                                                                      BIN1.006
       COMMON /BIN1/ NW, NX, XL(20), Z(20), U(20,20)                   BIN1.007
C                                                                      BIN1.008
       DATA NW /5/                                                     BIN1.009
       DATA NX /5/                                                     BIN1.010
       DATA XL / 2.5E-6, 10.E-6, 40.E-6, 160.E-6, 640.E-6, 15*0. /     BIN1.011
       DATA  Z /1.0,   .75,   .5,   .25,   0.,  15*0. /                BIN1.012
       DATA  U / .187, .405, .372, .144, .005,        15*0.,           BIN1.013
      X          .208, .554, .639, .337, .026,        15*0.,          BIN1.014
      X          .232, .799,1.346, .959, .164,        15*0.,          BIN1.015
      X          .260,1.237, 0.  , 0.  , 0.   ,       15*0.,          BIN1.016
      X          .294,2.121, 0.,   0.,     0.,        15*0. ,         BIN1.017
      X 300*0. /                                                       BIN1.018
       END                                                             BIN1.019
```

```
$IBFTC BDR.                                                    BDR.0001
      BLOCK DATA                                               BDR.0002
C     X IS R**2                                                BDR.0003
C                                                              BDR.0004
      COMMON /BLOCKR/ X(20)                                    BDR.0005
      DATA  X / 36.548312,                                     BDR.0006
     X          39.358308,                                     BDR.0007
     X          42.272363,                                     BDR.0008
     X          46.838556,                                     BDR.0009
     X          48.412651,                                     BDR.0010
     X          50.012759,                                     BDR.0011
     X          14*0.   /                                      BDR.0012
      END                                                      BDR.0013
```

```
$IBFTC BD.      DECK                                                    BD.00001
C                                                                       BD.00002
C       BLOCK DATA SUBPROGRAM FOR 122 CO VALUES AND 7 W2 VALUES         BD.00003
C                                                                       BD.00004
        BLOCK DATA                                                      BD.00005
C                                                                       BD.00006
        COMMON /BLOCKW/ W2(20)                                          BD.00007
        COMMON /BLOCKC/ CO(160)                                         BD.00008
C                                                                       BD.00009
        DATA W2                                                         BD.00010
       1/416930.0, 583702.0, 817182.8, 1144056., 1601678., 2242349.,    BD.00011
       23139289., 13*0.     /                                          BD.00012
C                                                                       BD.00013
        DATA  CO                                                        BD.00014
       1/.170E-5, .350E-5, .530E-4, .115E-3, .850E-4, .550E-4, .310E-4, BD.00015
       2 .750E-5, .700E-5, .650E-5, .820E-5, .100E-4, .135E-4, .170E-4, BD.00016
       3 .260E-4, .340E-4, .360E-4, .370E-4, .300E-4, .225E-4, .215E-4, BD.00017
       4 .205E-4, .301E-4, .400E-4, .435E-4, .470E-4, .410E-4, .350E-4, BD.00018
       5 .280E-4, .210E-4, .225E-4, .235E-4, .245E-4, .260E-4, .258E-4, BD.00019
       6 .255E-4, .245E-4, .235E-4, .225E-4, .210E-4, .205E-4, .200E-4, BD.00020
       7 .310E-4, .420E-4, .440E-4, .420E-4, .380E-4, .340E-4, .300E-4, BD.00021
       8 .260E-4, .255E-4, .250E-4, .245E-4, .240E-4, .232E-4, .225E-4, BD.00022
       9 .215E-4, .205E-4, .190E-4, .170E-4, .163E-4, .155E-4, .175E-4, BD.00023
       X .190E-4, .225E-4, .260E-4, .240E-4, .220E-4, .195E-4, .190E-4, BD.00024
       1 .182E-4, .175E-4, .170E-4, .165E-4, .160E-4, .150E-4, .140E-4, BD.00025
       2 .130E-4, .110E-4, .900E-5, .650E-5, .450E-5, .500E-5, .550E-5, BD.00026
       3 .820E-5, .110E-4, .113E-4, .115E-4, .920E-5, .700E-5, .600E-5, BD.00027
       4 .500E-5, .400E-5, .300E-5, .230E-5, .150E-5, .100E-5, .150E-5, BD.00028
       5 .220E-5, .300E-5, .400E-5, .500E-5, .470E-5, .450E-5, .420E-5, BD.00029
       6 .400E-5, .500E-5, .600E-5, .680E-5, .750E-5, .700E-5, .650E-5, BD.00030
       7 .580E-5, .500E-5, .420E-5, .350E-5, .300E-5, .200E-5, .150E-5, BD.00031
       8 .100E-5, .500E-6, .0, 0., 0., 36*0.                       /    BD.00032
        END                                                             BD.00033
```

```
*IBFTC BD.      DECK                                                          BD.00001
C                                                                             BD.00002
C       BLOCK DATA SUBPROGRAM FOR 160 CO VALUES AND 7 W2 VALUES               BD.00003
C                                                                             BD.00004
        BLOCK DATA                                                            BD.00005
C                                                                             BD.00006
        COMMON /BLOCKW/ W2(20)                                                BD.00007
        COMMON /BLOCKC/ CO(160)                                               BD.00008
C                                                                             BD.00009
        DATA W2                                                               BD.00010
       1/416930.0, 583702.0, 817182.8, 1144056., 1601678., 2242349.,          BD.00011
       2)139289., 13*0.    /                                                 BD.00012
C                                                                             BD.00013
        DATA (CO(I),I=1,114)                                                  BD.00014
       1/.65000E-5,.90000E-5,.11000E-4,.13250E-4,.16000E-4,.19250E-4,         BD.00015
       2 .23250E-4,.28000E-4,.33500E-4,.40000E-4,.47750E-4,.56750E-4,         BD.00016
       3 .67250E-4,.79500E-4,.93750E-4,.11025E-3,.12925E-3,.15150E-3,         BD.00017
       4 .17700E-3,.20600E-3,.23925E-3,.27725E-3,.32050E-3,.36975E-3,         BD.00018
       5 .42525E-3,.48775E-3,.55825E-3,.63725E-3,.72575E-3,.82450E-3,         BD.00019
       6 .93425E-3,.105575E-2,.119025E-2,.133875E-2,.150175E-2,.168025E-2,BD.00020
       7 .18755E-2,.208825E-2,.231925E-2,.256950E-2,.283950E-2,.313025E-2,BD.00021
       8 .34420E-2,.377525E-2,.413075E-2,.450825E-2,.490775E-2,.532950E-2,BD.00022
       9.577325E-2,.623825E-2,.672375E-2,.722900E-2,.775275E-2,.829375E-2,BD.00023
       X.885050E-2,.942100E-2,.01000325 ,.01059475 ,.01119325 ,.01179625 ,BD.00024
       1.01240075 ,.01300375 ,.01360175 ,.01419175 ,.01477075 ,.01533475 ,BD.00025
       2.01588050 ,.01640475 ,.01690400 ,.01737525 ,.01781500 ,.01822000 ,BD.00026
       3.01858775 ,.01891575 ,.01920150 ,.01944275 ,.01963800 ,.01978575 ,BD.00027
       4.01988475 ,.01993450 ,.01993450 ,.01988475 ,.01978575 ,.01963800 ,BD.00028
       5.01944275 ,.01920150 ,.01891575 ,.01858775 ,.01822000 ,.01781500 ,BD.00029
       6.01737525 ,.01690400 ,.01640475 ,.01588050 ,.01533475 ,.01477075 ,BD.00030
       7.01419175 ,.01360175 ,.01300375 ,.01240075 ,.01179625 ,.01119325 ,BD.00031
       8.01059475 ,.01000325 ,.00942010 ,.00885050 ,.00829375 ,.00775275 ,BD.00032
       9.00722900 ,.00672375 ,.00623825 ,.00577325 ,.00532950 ,.00490775 /BD.00033
        DATA (CO(I),I=115,160)                                                BD.00034
       1/.00450825,.00413075 ,.00377525 ,.00344200 ,.00313025 ,.00283950 ,BD.00035
       2.002569500,.00231925 ,.00208825 ,.00187550 ,.00168025 ,.00150175 ,BD.00036
       3.001338750,.00119025 ,.00105575 ,.934250E-3,.824500E-3,.725750E-3,BD.00037
       4.637250E-3,.558250E-3,.487750E-3,.425250E-3,.369750E-3,.320050E-3,BD.00038
       5.277250E-3,.239250E-3,.206000E-3,.177000E-3,.151500E-3,.129250E-3,BD.00039
       6.110250E-3,.937500E-4,.795000E-4,.672500E-4,.567500E-4,.477500E-4,BD.00040
       7.400000E-4,.335000E-4,.280000E-4,.232500E-4,.192500E-4,.160000E-4,BD.00041
       8.132500E-4,.110000E-4,.900000E-5,.650000E-5 /                         BD.00042
        END                                                                   BD.00043
```

```
$IBFTC BD.      DECK                                                    BD.00001
C                                                                       BD.00002
C       BLOCK DATA SUBPROGRAM FOR 32 CO VALUES AND 7 W2 VALUES          BD.00003
C                                                                       BD.00004
        BLOCK DATA                                                      BD.00005
C                                                                       BD.00006
        COMMON /BLOCKW/ W2(20)                                          BD.00007
        COMMON /BLOCKC/ C0(160)                                         BD.00008
C                                                                       BD.00009
        DATA W2                                                         BD.00010
       1/416930.0, 583702.0, 817182.8, 1144056., 1601678., 2242349.,    BD.00011
       23139289., 13*0.    /                                           BD.00012
C                                                                       BD.00013
        DATA C0                                                         BD.00014
       1/.9132400E-3, .3044140E-2, .6392700E-2, .1053272E-1, .1497716E-1 BD.00015
       2,.2051750E-1, .2538812E-1, .3031964E-1, .3494672E-1, .3975646E-1 BD.00016
       3,.4383562E-1, .4706240E-1, .4968036E-1, .5144596E-1, .5296804E-1 BD.00017
       4,.5382040E-1, .5461188E-1, .5467276E-1, .5418570E-1, .5333334E-1 BD.00018
       5,.5144596E-1, .4858448E-1, .4407914E-1, .3835616E-1, .3117200E-1 BD.00019
       6,.2496194E-1, .1960426E-1, .1503806E-1, .1120244E-1, .7427700E-2 BD.00020
       7,.4322599E-2, .8140020E-4, 128*0. /                             BD.00021
        END                                                             BD.00022
```

```
$IBMAP RAND.    100,DECK                                        RAND.001
*               GENERATES UNIFORM RANDOM NUMBERS                RAND.002
*               R=FLRAN(Y), Y DUMMY GIVES REAL NUMBER           RAND.003
*               CALL SAVE(Z) GIVES LAST OCTAL VALUE             RAND.004
*               CALL VALUE(Z) GIVES STARTING OCTAL VALUE        RAND.005
        ENTRY   FLRAN                                           RAND.006
        ENTRY   SAVE                                            RAND.007
        ENTRY   VALUE                                           RAND.008
 FLRAN  LDQ     RANDOM                                          RAND.009
        MPY     GENERA                                          RAND.010
        STO     RANDOM                                          RAND.011
        CLA     AAA                                             RAND.012
        LGL     28                                              RAND.013
        FAD     AAA                                             RAND.014
        TRA     1,4                                             RAND.015
 VALUE  CLA*    3,4                                             RAND.016
        STO     RANDOM                                          RAND.017
        TRA     1,4                                             RAND.018
 SAVE   CLA     RANDOM                                          RAND.019
        STO*    3,4                                             RAND.020
        TRA     1,4                                             RAND.021
RANDOM  OCT     343277244615                                    RAND.022
AAA     OCT     172000000100                                    RAND.023
GENERA  OCT     343277244615                                    RAND.024
        END                                                     RAND.025
```

```
$IBFTC PLOTR.  DECK                                                    PLOTR.01
       SUBROUTINE PLOTR                                                PLOTR.02
       COMMON  SCH(4), SCF(4)                                          PLOTR.03
       COMMON /PLTR/ PDATA(438), IPLTS, HEAD(12)                       PLOTR.04
       COMMON /BINP1/ DH, H, NC, F(162), CM(162) , SKIP2               PLOTR.05
       COMMON /BLPS/ N, NM, BF(1000), BM(1000), K                      PLOTR.06
       COMMON /BIN2/ USEIN2                                            PLOTR.07
       DATA HTITLE /1HM/, FTITLE /4HF(M)/                              PLOTR.08
       LOGICAL SKIP2                                                   PLOTR.09
       LOGICAL  USEIN2                                                 PLOTR.10
       IF ( SKIP2 )  RETURN                                            PLOTR.11
       IF ( .NOT. USEIN2 )  GO TO 7                                    PLOTR.12
       SCH(1) = BM(1)                                                  PLOTR.13
       SCH(2) = BM(K)                                                  PLOTR.14
       GO TO 8                                                         PLOTR.15
     7 DM = DH/H                                                       PLOTR.16
       DO 5 I = 1,NC                                                   PLOTR.17
     5 F(I) = F(I) / DM                                                PLOTR.18
       SCH(1) = AMIN1( CM(1), BM(1) )                                  PLOTR.19
       SCH(2) = AMAX1( CM(NC), BM(K) )                                 PLOTR.20
     8 SCF(1) = 0.                                                     PLOTR.21
       SCF(2) = 0.                                                     PLOTR.22
       IF ( USEIN2 )  GO TO 15                                         PLOTR.23
       DO 10 I = 1,NC                                                  PLOTR.24
    10 SCF(2) = AMAX1( SCF(2), F(I) )                                  PLOTR.25
    15 DO 20 I = 1,K                                                   PLOTR.26
    20 SCF(2) = AMAX1( SCF(2), BF(I) )                                 PLOTR.27
       CALL SCALE (SCH, 15., 2, 1, 10. )                               PLOTR.28
       CALL SCALE (SCF, 10., 2, 1, 10. )                               PLOTR.29
       IF ( USEIN2 )  GO TO 25                                         PLOTR.30
       CM(NC+1) = SCH(3)                                               PLOTR.31
       CM(NC+2) = SCH(4)                                               PLOTR.32
       F(NC+1)  = SCF(3)                                               PLOTR.33
       F(NC+2)  = SCF(4)                                               PLOTR.34
    25 BM(K+1) = SCH(3)                                                PLOTR.35
       BM(K+2) = SCH(4)                                                PLOTR.36
       BF(K+1) = SCF(3)                                                PLOTR.37
       BF(K+2) = SCF(4)                                                PLOTR.38
       CALL PLOT ( 5., -11., -3 )                                      PLOTR.39
       CALL PLOT ( 0.,  .5 , -3 )                                      PLOTR.40
       CALL AXIS ( 0., 0., HTITLE, -1, 16., 0., SCH(3), SCH(4), 10. )  PLOTR.41
       CALL AXIS ( 0., 0., FTITLE,  4, 10.,90., SCF(3), SCF(4), 10. )  PLOTR.42
       CALL SYMBOL ( 1., 9.5, .25, HEAD, 0., 72 )                      PLOTR.43
       IF ( .NOT. USEIN2 )  CALL LINE ( CM, F, NC, 1, 0, 0 )           PLOTR.44
       CALL LINE ( BM, BF, K, 1, 1, 1 )                                PLOTR.45
       CALL PLOT ( 15., 0., -3 )                                       PLOTR.46
       IPLTS = IPLTS + 1                                               PLOTR.47
       RETURN                                                          PLOTR.48
       END                                                             PLOTR.49
```

```
$IBFTC ORDER.  DECK                                                    ORDER.01
       SUBROUTINE ORDER ( X, Y, NM, N, K )                             ORDER.02
       COMMON  /PRTCTL/ WRITE                                          ORDER.03
       DIMENSION X(1), Y(1)                                            ORDER.04
       LOGICAL  WRITE                                                  ORDER.05
       J = 0                                                           ORDER.06
       DO 10 LN = 1,N                                                  ORDER.07
       N20 = (LN-1) * 20                                               ORDER.08
       L = N20 + 1                                                     ORDER.09
       J = J + 1                                                       ORDER.10
       X(J) = X(L)                                                     ORDER.11
       Y(J) = Y(L)                                                     ORDER.12
       DO 10 I = 2,NM                                                  ORDER.13
       L = N20 + I                                                     ORDER.14
       J = J + 1                                                       ORDER.15
       X(J) = X(L)                                                     ORDER.16
    10 Y(J) = Y(L)                                                     ORDER.17
       K = J                                                           ORDER.18
    20 TEST = 0.                                                       ORDER.19
       DO 30 I =2,J                                                    ORDER.20
       IF ( X(I-1) .LE. X(I) )  GO TO 30                               ORDER.21
       XS = X(I-1)                                                     ORDER.22
       YS = Y(I-1)                                                     ORDER.23
       X(I-1) = X(I)                                                   ORDER.24
       Y(I-1) = Y(I)                                                   ORDER.25
       X(I) = XS                                                       ORDER.26
       Y(I) = YS                                                       ORDER.27
       TEST = 1.                                                       ORDER.28
    30 CONTINUE                                                        ORDER.29
       IF ( (TEST .EQ. 0.) .OR. ( J .EQ. 2 ) )  GO TO 40               ORDER.30
       J = J - 1                                                       ORDER.31
       GO TO 20                                                        ORDER.32
    40 IF ( WRITE ) WRITE (6,600) (I, X(I), Y(I), I=1,K )              ORDER.33
       RETURN                                                          ORDER.34
   600 FORMAT         ( 1H1, 15X, 1HM, 19X, 1HF / 1H /                 ORDER.35
      X                                          ( 1X, I3, 2E20.7 ) )  ORDER.36
       END                                                             ORDER.37
```

```
$IBFTC DETA.   DECK                                                    DETA.001
       SUBROUTINE DETA ( A, B, NM, NROW )                              DETA.002
       COMMON  /PRTCTL/ WRITE                                          DETA.003
       DIMENSION A(51,120), B(NM,NM)                                   DETA.004
       LOGICAL  WRITE                                                  DETA.005
       IF ( WRITE )  WRITE (6,600)                                     DETA.006
       J = 1                                                           DETA.007
    10 DO 20 I = 1,NM                                                  DETA.008
       DO 20 K = 1,NM                                                  DETA.009
       JI = J + I                                                      DETA.010
    20 B(I,K) = A(JI,K)                                                DETA.011
       D = DET ( B, NM )                                               DETA.012
       IF ( WRITE )  WRITE (6,601) J, D                                DETA.013
       J = J + NM                                                      DETA.014
       IF ( (J+NM-1) .GT. NROW )  RETURN                               DETA.015
       GO TO 10                                                        DETA.016
   600 FORMAT ( 13HODETERMINANTS )                                     DETA.017
   601 FORMAT ( 3X, I4, E19.7 )                                        DETA.018
       END                                                             DETA.019
```

```
$IBFTC DLETE.  DECK                                                    DLETE001
       SUBROUTINE DLETE ( IRHS, NROW, NRP1, NCOL, NM, * )              DLETE002
       COMMON  JRHS(100)                                               DLETE003
       COMMON /BIN1/ NW, NX, XL(2)), Z(20), U(20,20)                   DLETE004
       COMMON /DLT/  NWW, NXX                                          DLETE005
       COMMON  /PRTCTL/ WRITE                                          DLETE006
       LOGICAL WRITE                                                   DLETE007
       KRHS = 2 * IRHS                                                 DLETE008
       IF ( KRHS .GT. 100 )  GO TO 900                                 DLETE009
       READ (5,500) (JRHS(I),I=1,KRHS)                                 DLETE010
       IF ( WRITE )  WRITE (6,601) IRHS, (JRHS(I),I=1,KRHS)            DLETE011
       DO 10 I = 1,KRHS,2                                              DLETE012
       K = JRHS(I)                                                     DLETE013
       L = JRHS(I+1)                                                   DLETE014
    10 U(K,L) = 0.                                                     DLETE015
       NWW = NW                                                        DLETE016
       I = 0                                                           DLETE017
       DO 30 K = 1,NW                                                  DLETE018
       USUM = 0.                                                       DLETE019
       DO 20 L = 1,NX                                                  DLETE020
    20 USUM = USUM + U(K,L)                                            DLETE021
       IF ( USUM .EQ. 0. )  GO TO 28                                   DLETE022
       I = I + 1                                                       DLETE023
       DO 25 J = 1,NX                                                  DLETE024
    25 U(I,J) = U(K,J)                                                 DLETE025
       XL(I) = XL(K)                                                   DLETE026
       GO TO 30                                                        DLETE027
    28 NWW = NWW- 1                                                    DLETE028
    30 CONTINUE                                                        DLETE029
       NXX = NX                                                        DLETE030
       J = 0                                                           DLETE031
       DO 50 L = 1,NX                                                  DLETE032
       USUM = 0.                                                       DLETE033
       DO 40 K = 1,NWW                                                 DLETE034
    40 USUM = USUM + U(K,L)                                            DLETE035
       IF ( USUM .EQ. 0. )  GO TO 48                                   DLETE036
       J = J + 1                                                       DLETE037
       DO 45 I = 1,NWW                                                 DLETE038
    45 U(I,J) = U(I,L)                                                 DLETE039
       Z(J) = Z(L)                                                     DLETE040
       GO TO 50                                                        DLETE041
    48 NXX = NXX - 1                                                   DLETE042
    50 CONTINUE                                                        DLETE043
       NROW = NXX * NWW                                                DLETE044
       NRP1 = NROW + 1                                                 DLETE045
       NCOL = NM + (2*NROW)                                            DLETE046
       IF ( .NOT. WRITE )  RETURN                                      DLETE047
       WRITE (6,602)  NWW, NXX                                         DLETE048
       DO 60 I = 1,NWW                                                 DLETE049
    60 WRITE (6,603) I, (U(I,J),J=1,NXX)                               DLETE050
       RETURN                                                          DLETE051
   900 WRITE (6,600) IRHS                                              DLETE052
       RETURN 1                                                        DLETE053
   500 FORMAT ( 27( 2I1,1X) )                                          DLETE054
   600 FORMAT ( 45HONUMBER OF U MATRIX DELETIONS GREATER THAN 50 /     DLETE055
      X          7H0IRHS = I4 )                                       DLETE056
   601 FORMAT ( 1HA, I3, 41H ELEMENTS OF MATRIX -U- HAVE BEEN DELETED / DLETE057
      X            33(2X,2I1) )                                       DLETE058
   602 FORMAT ( 20HAU MATRIX (ADJUSTED), I10, 5H ROWS, I6, 8H COLUMNS ) DLETE059
   603 FORMAT ( 4H0ROW, I4, 1X, 6E20.7 / (9X, 6E20.7) )                DLETE060
       END                                                             DLETE061
```

```
$IBFTC LPS.     DECK                                                    LPS.0001
       SUBROUTINE LPS ( * )                                             LPS.0002
       COMMON  IE(20), E(51,51), X(51), P(51), Y(51), JH(51),           LPS.0003
      X          KB(120), KOUT(7), ERR(8)                              LPS.0004
       COMMON /BIN1/  NW, NX, XL(20), Z(20), U(20,20)                   LPS.0005
       COMMON /BLPS/ N, NM, BF(20,50), BM(20,50), K                     LPS.0006
       COMMON /DLT/  NWW, NXX                                           LPS.0007
       COMMON  /PRTCTL/ WRITE                                           LPS.0008
       DIMENSION A(51,120), B(51), INFIX(8), TOL(4), BA(400)            LPS.0009
       DIMENSION ABR(50), BS(51)                                        LPS.0010
       LOGICAL  WRITE                                                   LPS.0011
       DATA NMAX/50/, NMMAX/20/, NCOLMX/120/, NROWMX/50/                LPS.0012
       NAME LIST  /LP/ XM11, G, NM, N, IRHS,PERT                        LPS.0013
       PERT = 0.                                                        LPS.0014
       IRHS = 0                                                         LPS.0015
       READ (5,LP)                                                      LPS.0016
       IF ( WRITE )  WRITE (6,600)  XM11, G, NM, N                      LPS.0017
       IF ( N .GT. NMAX )  GO TO 900                                    LPS.0018
       IF ( NM .GT. NMMAX )  GO TO 904                                  LPS.0019
       NROW = NW * NX                                                   LPS.0020
       IF ( NROW .GT. NROWMX )  GO TO 902                               LPS.0021
       NCOL = NM + (2*NROW)                                             LPS.0022
       IF ( NCOL .GT. NCOLMX )  GO TO 901                               LPS.0023
       NRP1 = NROW + 1                                                  LPS.0024
       NWW = NW                                                         LPS.0025
       NXX = NX                                                         LPS.0026
       IF ( IRHS .GT. 0 )                                               LPS.0027
      X    CALL DLETE ( IRHS, NROW, NRP1, NCOL, NM, $903 )              LPS.0028
   20  DO 30 I = 1,NRP1                                                 LPS.0029
       DO 30 J = 1,NCOL                                                 LPS.0030
   30  A(I,J) = 0.                                                      LPS.0031
       DO 35 I = 1,NMMAX                                                LPS.0032
       DO 35 J = 1,NMAX                                                 LPS.0033
   35  BF(I,J) = 0.                                                     LPS.0034
       INFIX(1) = 4                                                     LPS.0035
       INFIX(2) = NCOL                                                  LPS.0036
       INFIX(3) = 51                                                    LPS.0037
       INFIX(4) = NRP1                                                  LPS.0038
       INFIX(5) = 2                                                     LPS.0039
       INFIX(6) = 1                                                     LPS.0040
       INFIX(7) = 500                                                   LPS.0041
       INFIX(8) = 20                                                    LPS.0042
       TOL(1)   = 1.E-7                                                 LPS.0043
       TOL(2)   = 1.E-7                                                 LPS.0044
       TOL(3) = 1.E-6                                                   LPS.0045
       TOL(4) = 1.E-10                                                  LPS.0046
       PRM = 0.                                                         LPS.0047
       B(1) = 0.                                                        LPS.0048
       DO 50 I = 1,NROW                                                 LPS.0049
       IN = (I-1) / NXX                                                 LPS.0050
       K  = IN + 1                                                      LPS.0051
       L =  I- (IN*NXX)                                                 LPS.0052
       B(I+1) = U(K,L)                                                  LPS.0053
       IF ( PERT .GT. 0. )  B(I+1) = B(I+1)*(1.+2.*PERT*(FLRAN(X)-.5))  LPS.0054
   50  BS(I+1) = B(I+1)                                                 LPS.0055
       LN = 1                                                           LPS.0056
       SQRTG = SQRT( G )                                                LPS.0057
       GMG = SQRTG - (1. / SQRTG)                                       LPS.0058
       XN = 1. / FLOAT(N)                                               LPS.0059
       BM(1,1) = XM11                                                   LPS.0060
       NROWS = NROW                                                     LPS.0061
```

```
 55 IF ( WRITE )  WRITE (6,612)  LN, N                                  LPS.0062
    NROW = NROWS                                                        LPS.0063
    NRP1 = NROW + 1                                                     LPS.0064
    DO 60 J = 1,NM                                                      LPS.0065
    BM(J,LN) = BM(1,LN)* G**(J-1)                                       LPS.0066
    DBM = GMG * BM(J,LN)                                                LPS.0067
    DO 60 I = 1,NROW                                                    LPS.0068
    IN = (I-1) / NXX                                                    LPS.0069
    K  = IN +1                                                          LPS.0070
    L =  I- (IN*NXX)                                                    LPS.0071
    XLKM = XL(K) * BM(J,LN)                                             LPS.0072
    XNUM = XLKM**2 * EXP( -XLKM * Z(L) )                                LPS.0073
    DENOM= 1. - EXP( -XLKM )                                            LPS.0074
 60 A(I+1,J) = (XNUM / DENOM) * DBM                                     LPS.0075
    II = 1                                                              LPS.0076
    DO 64 I = 2,NRP1                                                    LPS.0077
    B(I) = BS(I)                                                        LPS.0078
    IF ( B(I) .EQ. 0. )  GO TO 64                                       LPS.0079
    II = II + 1                                                         LPS.0080
    B(II) = B(I)                                                        LPS.0081
    DO 62 J = 1,NM                                                      LPS.0082
 62 A(II,J) = A(I,J)                                                    LPS.0083
 64 CONTINUE                                                            LPS.0084
    NRP1 = II                                                           LPS.0085
    NROW = NRP1 - 1                                                     LPS.0086
    INFIX(4) = NRP1                                                     LPS.0087
    J = NM                                                              LPS.0088
    DO 68 I = 2,NRP1                                                    LPS.0089
    J = J + 1                                                           LPS.0090
    A(1,J) = 1.0                                                        LPS.0091
    A(I,J) = 1.0                                                        LPS.0092
    J = J + 1                                                           LPS.0093
    A(1,J) = 1.0                                                        LPS.0094
 68 A(I,J) = -1.0                                                       LPS.0095
    CALL DETA ( A, BA, NM, NROW )                                       LPS.0096
    IF ( WRITE )  WRITE (6,601) (M,M=1,30)                              LPS.0097
    DO 80 I = 2,NRP1                                                    LPS.0098
    DO 70 J = 1,NM                                                      LPS.0099
    IF(J) = -99                                                         LPS.0100
 70 IF ( A(I,J) .NE. 0. )  IF(J) = ALOG10( A(I,J) )                     LPS.0101
    IM1 = I - 1                                                         LPS.0102
 80 IF ( WRITE )  WRITE (6,602)  IM1, (IF(J),J=1,NM)                    LPS.0103
    CALL SIMPLX ( INFIX, A, B, TOL, PRM, KOUT, ERR, JH, X, P, Y,KB,E )LPS.0104
    IF ( WRITE )  WRITE (6,603)                                         LPS.0105
    DO 90 J = 1,NRP1                                                    LPS.0106
    MX = JH(J)                                                          LPS.0107
 90 IF ( (MX .GT. 0) .AND. (MX .LE. NM) )  BF(MX,LN) = X(J)             LPS.0108
    ABR(LN) = 0.                                                        LPS.0109
    DO 110 I = 2,NRP1                                                   LPS.0110
    BC = 0.                                                             LPS.0111
    DO 100 J = 1,NM                                                     LPS.0112
100 BC = BC + BF(J,LN) * A(I,J)                                         LPS.0113
    BD = B(I) - BC                                                      LPS.0114
    AB = ABS( BD ) / B(I)                                               LPS.0115
    IF ( WRITE )  WRITE (6,604)  B(I), BC, BD, AB                       LPS.0116
110 ABR(LN) = ABR(LN) + AB                                              LPS.0117
    ABR(LN) = ABR(LN) / FLOAT( NROW )                                   LPS.0118
    IF ( .NOT. WRITE )  GO TO 115                                       LPS.0119
    WRITE (6,605) ABR(LN)                                               LPS.0120
    WRITE (6,606) LN, (BF(M,LN),M=1,NM)                                 LPS.0121
    WRITE (6,610)                                                       LPS.0122
```

```
115 LN = LN + 1                                                          LPS.0123
    IF ( LN .GT. N ) GO TO 120                                           LPS.0124
    BM(1,LN) = BM(1,LN-1) * G**XN                                        LPS.0125
    GO TO 55                                                             LPS.0126
120 IF ( WRITE )  WRITE (6,610)                                          LPS.0127
    WRITE (6,615)                                                        LPS.0128
    ARBAVG = 0.                                                          LPS.0129
    DO 130 I = 1,N                                                       LPS.0130
    ARBAVG = ARBAVG + ABR(I)                                             LPS.0131
130 WRITE (6,614)  I, ABR(I), (BF(M,I),M=1,NM)                           LPS.0132
    ARBAVG = ARBAVG / FLOAT( N )                                         LPS.0133
    WRITE (6,613) ARBAVG                                                 LPS.0134
    CALL ORDER ( BM, BF, NM, N, K )                                      LPS.0135
    RETURN                                                               LPS.0136
900 WRITE (6,607) N                                                      LPS.0137
    RETURN 1                                                             LPS.0138
901 WRITE (6,608) NCOL                                                   LPS.0139
    RETURN 1                                                             LPS.0140
902 WRITE (6,609) NROW                                                   LPS.0141
903 RETURN 1                                                             LPS.0142
904 WRITE (6,611) NM                                                     LPS.0143
    RETURN 1                                                             LPS.0144
600 FORMAT ( 33HAFIRST MOLECULAR WEIGHT          = E16.7  /              LPS.0145
   X          33H MOLECULAR WEIGHT MULTIPLIER    = E16.7  /              LPS.0146
   X          33H NUMBER OF MOLECULAR WT. VALUES = I8     /              LPS.0147
   X          33H NUMBER OF LP SETS FOR SOLUTION = I8     )              LPS.0148
601 FORMAT ( 1HA, 57X, 14HA MATRIX (LOG) / 1H0, 60X, 7HCOLUMNS /         LPS.0149
   X          5H ROWS, 30I4 / 1H )                                       LPS.0150
602 FORMAT ( 1X, I3, 1X, 30I4 / ( 5X, 30I4 ) )                           LPS.0151
603 FORMAT ( 1H1, 7X, 9HINPUT RHS, 7X, 12HCOMPUTED RHS, 6X,              LPS.0152
   X                14HRHS DIFFERENCE, 4X, 16HABS REL DIFF RHS / 1H )LPS.0153
604 FORMAT ( 1X, 4E18.7 )                                                LPS.0154
605 FORMAT ( 34H0AVERAGE RELATIVE DIFFERENCE RHS = E16.7 )               LPS.0155
606 FORMAT ( 9H0SOLUTION, I4, 7X, 7E16.7 / (20X, 7E16.7) )               LPS.0156
607 FORMAT ( 4H0N = I4, 42H IS GREATER THAN DIMENSION FOR NO. OF SETS)LPS.0157
608 FORMAT ( 56H0NUMBER OF COLUMNS FOR -A- MATRIX GREATER THAN DIMENSILPS.0158
   XON    /  7H0NROW = I4 )                                              LPS.0159
609 FORMAT ( 53H0NUMBER OF ROWS FOR -A- MATRIX GREATER THAN DIMENSION LPS.0160
   X          / 7H0ROW = I4 )                                           LPS.0161
610 FORMAT ( 1H1 )                                                       LPS.0162
611 FORMAT ( 5H0NM = I4, 59H IS GREATER THAN DIMENSION FOR NUMBER OF SLPS.0163
   XOLUTIONS PER SET )                                                   LPS.0164
612 FORMAT ( 1H0, 57X, 3HSET I3, 3H OF I3 )                              LPS.0165
613 FORMAT ( 1H0 / 20X, 38HTHE AVERAGE REL. DIFF. FOR ALL SETS IS        LPS.0166
   X          E16.7 )                                                   LPS.0167
614 FORMAT (  1H0, I4, E22.7, 9X, 6E16.7 / (36X, 6E16.7) )               LPS.0168
615 FORMAT (6H0  SET,6X,15HAVG. REL. ERROR,12X,11HSOLUTIONS ,82(1H*)     LPS.0169
   X     / 1H )                                                          LPS.0170
    END                                                                  LPS.0171
```

```
$IBFTC IN1.    DECK                                                    IN1.0001
      SUBROUTINE IN1 ( * )                                             IN1.0002
      COMMON  /BLOCKR/ X(20)                                           IN1.0003
      COMMON /BLOCKC/ C0(160)                                          IN1.0004
      COMMON /BLOCKW/ W2(20)                                           IN1.0005
      COMMON /BIN1/  NW, NX, XL(20), Z(20), U(20,20)                   IN1.0006
      COMMON /BIN2/ USEIN2                                             IN1.0007
      COMMON /BINP1/ DH, H, NC, F(162), H0(162), SKIP2                 IN1.0008
      COMMON  /PRTCTL/ WRITE                                           IN1.0009
C                                                                      IN1.0010
      DATA  NXMAX/20/, NHMAX/160/, NWMAX/20/                           IN1.0011
C                                                                      IN1.0012
      LOGICAL  WRITE, SKIP1, SKIP2                                     IN1.0013
      LOGICAL USEIN2                                                   IN1.0014
C                                                                      IN1.0015
      NAME LIST  /INP1/ NW, NX, H1, DH, NH, H, CZ, X1, DX,             IN1.0016
     X              IST, LST, LAST, WRITE, SKIP1, SKIP2, USEIN2       IN1.0017
C                                                                      IN1.0018
      WRITE =.FALSE.                                                   IN1.0019
      SKIP1 = .FALSE.                                                  IN1.0020
      SKIP2 = .FALSE.                                                  IN1.0021
      USEIN2 = .FALSE.                                                 IN1.0022
      LAST = 1                                                         IN1.0023
      READ (5,INP1)                                                    IN1.0024
      IF ( LAST .EQ. 0 )  RETURN 1                                     IN1.0025
      IF ( SKIP1 )  GO TO 75                                           IN1.0026
      IF ( NX .GT. NXMAX )  GO TO 900                                  IN1.0027
      IF ( NH .GT. NHMAX )  GO TO 901                                  IN1.0028
      IF ( NW .GT. NWMAX )  GO TO 902                                  IN1.0029
      IF ( USEIN2 )  CALL IN2 ( $85 )                                  IN1.0030
      NC = LST - IST + 1                                               IN1.0031
      IF ( NC .GT. NHMAX )  GO TO 903                                  IN1.0032
      IF ( X1 .LE. 0. )  GO TO 5                                       IN1.0033
      X(1) = X1                                                        IN1.0034
      DO 10 L = 2,NX                                                   IN1.0035
   10 X(L) = X1 + FLOAT(L-1) * DX                                      IN1.0036
    5 H0(1) = H1                                                       IN1.0037
      H0(1) = H1                                                       IN1.0038
      DO 20 N = 2,NH                                                   IN1.0039
   20 H0(N) = H1 + FLOAT(N-1) * DH                                     IN1.0040
      DO 30 I = 1,NC                                                   IN1.0041
      IC = I + IST - 1                                                 IN1.0042
      F(I)  = C0(IC) / CZ                                              IN1.0043
   30 H0(I) = H0(IC) / H                                               IN1.0044
      B = X(NX)                                                        IN1.0045
      BMM = B - X1                                                     IN1.0046
      DO 40 K = 1,NW                                                   IN1.0047
   40 XL(K) = BMM * H * W2(K)                                          IN1.0048
      DO 50 L = 1,NX                                                   IN1.0049
   50 Z(L) = (B - X(L)) / BMM                                          IN1.0050
      DO 70 K = 1,NW                                                   IN1.0051
      DO 70 L = 1,NX                                                   IN1.0052
      U(K,L) = 0.                                                      IN1.0053
      DO 70 N = 1,NC                                                   IN1.0054
      XLM = XL(K) * H0(N)                                              IN1.0055
      XNUM = XLM**2 * EXP( -XLM*Z(L) )                                 IN1.0056
      DENOM= 1. - EXP( -XLM )                                          IN1.0057
   70 U(K,L) = U(K,L) + ( XNUM / DENOM ) * F(N)                        IN1.0058
   75 IF ( .NOT. WRITE )  GO TO 85                                     IN1.0059
      WRITE (6,601) NW, (W2(K),K=1,NW)                                 IN1.0060
      WRITE (6,602) NX, (Z(L),L=1,NX)                                  IN1.0061
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```
      WRITE (6,603) NW, NX                                                IN1.0062
      DO 80 K = 1,NW                                                      IN1.0063
   80 WRITE (6,604) K, (U(K,L),L=1,NX)                                    IN1.0064
   85 RETURN                                                              IN1.0065
  900 WRITE (6,605) NX                                                    IN1.0066
      STOP                                                                IN1.0067
  901 WRITE (6,606) NH                                                    IN1.0068
      STOP                                                                IN1.0069
  902 WRITE (6,607) NW                                                    IN1.0070
      STOP                                                                IN1.0071
  903 WRITE (6,608) NC                                                    IN1.0072
      STOP                                                                IN1.0073
  601 FORMAT ( 1HA, I4, 40H VALUES OF ANGULAR VELOCITY SQUARED - W2 /     IN1.0074
     X         1H / ( 9X, 6E20.7 ) )                                      IN1.0075
  602 FORMAT ( 1HO, I4, 71H VALUES OF THE FUNCTION OF DISTANCE SQUARED FIN1.0076
     XROM CENTER OF ROTATION - Z  / 1H / ( 9X, 6E20.7 ) )                IN1.0077
  603 FORMAT ( 9HOU MATRIX, I10, 5H ROWS, I6, 8H COLUMNS )                IN1.0078
  604 FORMAT ( 4HOROW, I4, 1X, 6E20.7, / ( 9X, 6E20.7 ) )                 IN1.0079
  605 FORMAT ( 5HONX = I4, 33H IS GREATER THAN DIMENSION FOR X. )         IN1.0080
  606 FORMAT ( 5HONH = I4, 33H IS GREATER THAN DIMENSION FOR H. )         IN1.0081
  607 FORMAT ( 5HONW = I4, 37H IS GREATER THAN DIMENSION FOR OMEGA. )     IN1.0082
  608 FORMAT ( 5HONC = I4, 41H IS GREATER THAN DIMENSION FOR SELECTED H)IN1.0083
      END                                                                 IN1.0084
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$IBFTC IN2.    DECK                                                    IN2.0001
      SUBROUTINE IN2 ( * )                                            IN2.0002
C         SCRATCH STORAGE                                             IN2.0003
      COMMON DCDX(20,20)                                              IN2.0004
C                                                                     IN2.0005
      DIMENSION DNDR(20,20)                                           IN2.0006
C                                                                     IN2.0007
      LOGICAL  WRITE                                                  IN2.0008
C                                                                     IN2.0009
      COMMON  /BIN1 / NW, NR, XL(20), Z(20), U(20,20)                 IN2.0010
      COMMON /BLOCKW/  W2(20)                                         IN2.0011
      COMMON  /BLOCKR/ X(20)                                          IN2.0012
      COMMON  /PRTCTL/ WRITE                                          IN2.0013
C                                                                     IN2.0014
      DATA  NRMAX/20/, NWMAX/20/                                      IN2.0015
C                                                                     IN2.0016
      NAME LIST  /INP2/ NW, NR, H, C0, R1, DR, DCDN, DNDR, W2         IN2.0017
C                                                                     IN2.0018
      READ (5,INP2)                                                   IN2.0019
C                                                                     IN2.0020
      IF ( NR .GT. NRMAX )  GO TO 900                                 IN2.0021
      IF ( NW .GT. NWMAX )  GO TO 901                                 IN2.0022
C                                                                     IN2.0023
      DO 10 L = 1,NR                                                  IN2.0024
      IF ( R1 .LE. 0. )  GO TO 5                                      IN2.0025
      X(L) = ( R1 + FLOAT(L-1) * DR )**2                              IN2.0026
C                                                                     IN2.0027
    5 DO 10 K = 1,NW                                                  IN2.0028
   10 DCDX(K,L) = 1.0 / SQRT(X(L)) * DCDN * DNDR(K,L)                 IN2.0029
C                                                                     IN2.0030
      XM = X(1)                                                       IN2.0031
      B  = X(NR)                                                      IN2.0032
C                                                                     IN2.0033
      DO 20 K = 1, NW                                                 IN2.0034
   20 XL(K) = (B-XM) * H * W2(K)                                      IN2.0035
C                                                                     IN2.0036
      DO 30 L = 1, NR                                                 IN2.0037
   30 Z(L) = (B-X(L)) / (B-XM)                                        IN2.0038
C                                                                     IN2.0039
      DO 40 L = 1,NR                                                  IN2.0040
      DO 40 K = 1,NW                                                  IN2.0041
   40 U(K,L) =((B-XM) / C0) *  DCDX(K,L)                              IN2.0042
C                                                                     IN2.0043
      IF ( .NOT. WRITE )  GO TO 60                                    IN2.0044
C                                                                     IN2.0045
      WRITE (6,601)  NW, (W2(K),K=1,NW)                               IN2.0046
      WRITE (6,602)  NR, ( Z(L),L=1,NR)                               IN2.0047
      WRITE (6,603)  NW, NR                                           IN2.0048
      DO 50 K = 1,NW                                                  IN2.0049
   50 WRITE (6,604)  K, (U(K,L),L=1,NR)                               IN2.0050
C                                                                     IN2.0051
   60 RETURN 1                                                        IN2.0052
  900 WRITE (6,605) NR, NRMAX                                         IN2.0053
      STOP                                                            IN2.0054
  901 WRITE (6,606) NW, NWMAX                                         IN2.0055
      STOP                                                            IN2.0056
C                                                                     IN2.0057
  601 FORMAT ( 1HA, I4, 40H VALUES OF ANGULAR VELOCITY SQUARED - W2 /  IN2.0058
     X         1H / ( 9X, 6E20.7 ) )                                  IN2.0059
  602 FORMAT ( 1H0, I4, 71H VALUES OF THE FUNCTION OF DISTANCE SQUARED FIN2.0060
     XROM CENTER OF ROTATION - Z  / 1H / ( 9X, 6E20.7 ) )             IN2.0061
```

```
  603 FORMAT ( 9HOU MATRIX, I10, 5H ROWS, I6, 8H COLUMNS )                    IN2.0062
  604 FORMAT ( 4HOROW, I4, 1X, 6E20.7 / ( 9X, 6E20.7 ) )                      IN2.0063
  605 FORMAT ( 5HONR = I4, 33H IS GREATER THAN DIMENSION FOR X(,I2,2H).)      IN2.0064
  606 FORMAT ( 5HONW = I4, 33H IS GREATER THAN DIMENSION FOR W(,I2,2H).)      IN2.0065
C                                                                             IN2.0066
      END                                                                     IN2.0067
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$IBFTC DET.    DECK                                          L. B. FALL        DET.0001
      FUNCTION DET(A,N)                                                       DET.0002
C                                                                             DET.0003
C           DETERMINANT EVALUATING FUNCTION                                   DET.0004
C                                                                             DET.0005
C           FUNCTION DET(A,N) COMPUTES THE DETERMINANT                        DET.0006
C     OF THE N-TH ORDER MATRIX A, WHICH MUST BE                               DET.0007
C     DIMENSIONED A(N,N).  THE ORIGINAL MATRIX A                              DET.0008
C     IS NOT ALTERED.                                                         DET.0009
C                                                                             DET.0010
C     612 CELLS OF BLANK COMMON ARE USED                                      DET.0011
C                                                                             DET.0012
C     TO CHANGE DIMENSIONS, CHANGE DIMENSIONS OF ARRAYS B AND PIV,            DET.0013
C     AND ALSO CHANGE VALUE OF NMAX IN THE DATA STATEMENT.                    DET.0014
C                                                                             DET.0015
      DIMENSION   A(N,N)                                                      DET.0016
      COMMON   D, I, II, J, K, KCT, KFROM, KTO, NN, NPR, RLE, TPE             DET.0017
      COMMON   B(24,24), PIV(24)                                              DET.0018
      DATA   NMAX/ 24/                                                        DET.0019
C                                                                             DET.0020
C     TEST ARGUMENT N TO PREVENT OVERFLOWING BLANK COMMON                     DET.0021
C                                                                             DET.0022
      NN=N                                                                    DET.0023
      IF ( NN .GT. NMAX .OR. NN .LE. 0 )     GO TO 100                        DET.0024
C                                                                             DET.0025
C     MOVE INPUT MATRIX A TO SCRATCH MATRIX B                                 DET.0026
C                                                                             DET.0027
      DO 10 I=1,NN                                                            DET.0028
      DO 10 J=1,NN                                                            DET.0029
 10   B(I,J)=A(I,J)                                                           DET.0030
C                                                                             DET.0031
C     INITIALIZE DETERMINANT VALUE AND ROW INTERCHANGE COUNT                  DET.0032
C                                                                             DET.0033
      D=1.0                                                                   DET.0034
      KCT=0                                                                   DET.0035
C                                                                             DET.0036
C     PERFORM ELIMINATION ON N COLUMNS                                        DET.0037
C                                                                             DET.0038
      DO 90 I=1,NN                                                            DET.0039
C                                                                             DET.0040
C     SEARCH I-TH SUB-COLUMN FOR I-TH PIVOT ELEMENT                           DET.0041
C                                                                             DET.0042
      TPE=0.                                                                  DET.0043
      DO 30 II=I,NN                                                           DET.0044
      IF (ABS(B(II,I))-TPE) 30,20,20                                          DET.0045
 20   NPR=II                                                                  DET.0046
      TPE=ABS(B(II,I))                                                        DET.0047
 30   CONTINUE                                                                DET.0048
C                                                                             DET.0049
C     IF PIVOT ELEMENT IS ZERO, THEN DET(A,N)=0.0                             DET.0050
C                                                                             DET.0051
      IF (B(NPR,I)) 35,32,35                                                  DET.0052
 32   D=0.                                                                    DET.0053
      GO TO 95                                                                DET.0054
C                                                                             DET.0055
C     DIVIDE PIVOT ROW BY PIVOT ELEMENT                                       DET.0056
C                                                                             DET.0057
 35   DO 40 J=I,NN                                                            DET.0058
 40   PIV(J)=B(NPR,J)/B(NPR,I)                                                DET.0059
C                                                                             DET.0060
C     UPDATE THE PRODUCT OF PIVOT ELEMENTS AND SUM OF ROW INTERCHANGES        DET.0061
```

```
C                                                                       DET.0062
      D=D*B(NPR,I)                                                      DET.0063
      KCT=KCT+(NPR-I)                                                   DET.0064
C                                                                       DET.0065
C     ELIMINATE REMAINING ELEMENTS IN I-TH SUB-COLUMN                   DET.0066
C                                                                       DET.0067
      KTO=NN                                                            DET.0068
      KFROM=NN                                                          DET.0069
      DO 90 K=I,NN                                                      DET.0070
      IF (KFROM-NPR) 70,80,70                                           DET.0071
 70   RLE=-B(KFROM,I)                                                   DET.0072
      DO 75 J=I,NN                                                      DET.0073
 75   B(KTO,J)=B(KFROM,J)+RLE*PIV(J)                                    DET.0074
      KTO=KTO-1                                                         DET.0075
 80   KFROM=KFROM-1                                                     DET.0076
 90   CONTINUE                                                          DET.0077
C                                                                       DET.0078
C     IF TOTAL NO. OF ROW INTERCHANGES WAS ODD, THEN                    DET.0079
C     NEGATE THE PRODUCT OF THE PIVOT ELEMENTS                          DET.0080
C                                                                       DET.0081
 95   IF ( KCT .NE. 2*(KCT/2) )     D=-D                                DET.0082
      DET=D                                                             DET.0083
      RETURN                                                            DET.0084
C                                                                       DET.0085
C     GIVE ERROR MESSAGE FOR INCORRECT VALUE OF N                       DET.0086
C     AND RETURN TO SYSTEM VIA FXEM                                     DET.0087
C                                                                       DET.0088
 100  WRITE (6,1000) NN                                                 DET.0089
      CALL FXEM                                                         DET.0090
      RETURN                                                            DET.0091
C                                                                       DET.0092
 1000 FORMAT (3H0N=,I12,30H IS INCORRECT FOR FUNCTION DET)              DET.0093
      END                                                               DET.0094
```

```
$IBFTC MSUB    DECK                                                          MSUB.001
CMSUBJ       VERSION 1 OF  RS MSUB                                           MSUB.002
      SUBROUTINE SIMPLX (INFIX,A,B,TOL,PRM,KOUT,ERR,JH,X,P,Y,KB,E)           MSUB.003
C                                                                            MSUB.004
      DIMENSION INFIX(8),A(1),B(1),TOL(4),KOUT(7),ERR(8),JH(1),X(1),         MSUB.005
     1 P(1),Y(1),KB(1),E(1),ZZ(3), IOFIX(16) , TERR(8)                       MSUB.006
C                                                                            MSUB.007
      EQUIVALENCE  (INFLAG,IOFIX(1) ), (N , IOFIX(2) ) ,                     MSUB.008
     1            (ME,IOFIX(3) ),  (M,IOFIX(4)), (MF,IOFIX(5)),            MSUB.009
     2  (MC, IOFIX(6) ),  ( NCUT, IOFIX(7) ) , ( NVER, IOFIX(8) ),           MSUB.010
     3 ( K, IOFIX(9) ), (IIER, IOFIX(10) ), (INVC , IOFIX(11) ) ,            MSUB.011
     4 (NUMVR, IOFIX(12) ), ( NUMPV, IOFIX(13) ) ,                           MSUB.012
     5  (INFS, IOFIX(14)  ) , ( JT,  IOFIX(15) ) ,( LA  , IOFIX(16) ),       MSUB.013
     6 (ZZ(1),TPIV), (ZZ(2),TZERO),(ZZ(3),TCOST)                             MSUB.014
C                                                                            MSUB.015
C                          MOVE INPUTS  ...  ZERO OUTPUTS                    MSUB.016
      DO 1340  I= 1, 8                                                       MSUB.017
       TERR(I) = 0.0                                                         MSUB.018
      IOFIX(I+8)  =  0                                                       MSUB.019
 1340  IOFIX(I)  =  INFIX(I)                                                 MSUB.020
      LA   =   0                                                             MSUB.021
      DO 1308  I = 1 , 3                                                     MSUB.022
 1308 ZZ(I)  =  TOL(I)                                                       MSUB.023
      TCOST  =  -  ABS  (TCOST)                                              MSUB.024
      PMIX = PRM                                                             MSUB.025
      M2 = M**2                                                              MSUB.026
      INFS = 1                                                               MSUB.027
C                    CHECK FOR ILLEGAL INPUT                                 MSUB.028
      IF (N)  1304, 1304, 1371                                               MSUB.029
 1371  IF (M - MF ) 1304, 1304, 1372                                         MSUB.030
 1372  IF (MF - MC)  1304, 1304, 1373                                        MSUB.031
 1373  IF ( MC ) 1304 , 1304,  1374                                          MSUB.032
 1374  IF (ME - M ) 1304, 1375, 1375                                         MSUB.033
 1375 IF(  MOD (INFLAG, 4 )  - 1 )  1400,  1320,  100                       MSUB.034
C                                                                            MSUB.035
C                                                                            MSUB.036
C  NEW 1          STARTS PHASE ONE                                          MSUB.037
C*****SUBROUTINE NEW (M,N, JH, KB, A, B, MF, ME )                           MSUB.038
C                                                                            MSUB.039
C                                INITIATE                                    MSUB.040
 1400   DO 1401 I = 1, M                                                     MSUB.041
 1401 JH(I) = 0                                                              MSUB.042
C                   INSTALL SINGLETONS                                       MSUB.043
       KT  =  0                                                              MSUB.044
        DO 1402  J = 1, N                                                    MSUB.045
      KB(J) = 0                                                              MSUB.046
      MM  =  KT + MF                                                         MSUB.047
      LL  =  KT + M                                                          MSUB.048
C                               TALLY ENTRIES IN CONSTRAINTS                 MSUB.049
      KQ  = 0                                                                MSUB.050
      DO  1403 L = MM , LL                                                   MSUB.051
      IF (A(L)) 1404, 1403, 1404                                             MSUB.052
 1404 KQ = KQ+1                                                              MSUB.053
      LQ = L                                                                 MSUB.054
 1403   CONTINUE                                                            MSUB.055
C                               CHECK WHETHER J IS CANDIDATE                 MSUB.056
           IF (KQ - 1) 1402, 1405, 1402                                      MSUB.057
 1405 IA = LQ- KT                                                            MSUB.058
         IF ( JH(IA) ) 1402, 1406, 1402                                      MSUB.059
 1406 IF (A(LQ)*B(IA)) 1402, 1407, 1407                                      MSUB.060
C                               J IS CANDIDATE. INSTALL                      MSUB.061
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 1407 JH(IA) = J                                                        MSUB.062
      KB(J)  = IA                                                       MSUB.063
 1402 KT = KT + ME                                                      MSUB.064
C                                                                       MSUB.065
C**END OF NEW                                                           MSUB.066
C                                                                       MSUB.067
C                                                                       MSUB.068
 1320 CONTINUE                                                          MSUB.069
C                                                                       MSUB.070
C  VER 1          FORMS INVERSE FROM  KB                               MSUB.071
C*****SUBROUTINE VER ( A, B, JH, X, E, KB, Y, IOFIX, TPIV, M2  )       MSUB.072
C                                                                       MSUB.073
C                  INITIATE                                             MSUB.074
 1100 ASSIGN  1102  TO KPIV                                             MSUB.075
      ASSIGN  1114  TO KJMY                                             MSUB.076
      IF (LA)  1121, 1121, 1122                                         MSUB.077
 1121 INVC = 0                                                          MSUB.078
 1122 NUMVR   =  NUMVR  +1                                              MSUB.079
       DO 1101  I = 1, M2                                               MSUB.080
 1101 E(I)=0.                                                           MSUB.081
      MM=1                                                              MSUB.082
       DO 1113  I = 1, M                                                MSUB.083
      E(MM) =1.0                                                        MSUB.084
      X(I) = B(I)                                                       MSUB.085
 1113 MM = MM + M + 1                                                   MSUB.086
        DO 1110  I = MF, M                                              MSUB.087
      IF (JH(I)) 1111, 1110, 1111                                       MSUB.088
 1111 JH(I) = 12345                                                     MSUB.089
 1110 CONTINUE                                                          MSUB.090
      INFS = 1                                                          MSUB.091
C                 FORM INVERSE                                         MSUB.092
        DO 1102  JT= 1, N                                               MSUB.093
      IF ( KB(JT))  600 , 1102 , 600                                    MSUB.094
C 600 CALL  JMY  (JT, A, E, M, Y )                                      MSUB.095
C                       CHOOSE PIVOT                                    MSUB.096
 1114 TY = 0.                                                           MSUB.097
        DO 1104  I = MF, M                                              MSUB.098
      IF (JH(I)  - 12345 )  1104, 1105, 1104                            MSUB.099
 1105 IF ( ABS ( Y(I) ) -  TY )  1104, 1104, 1106                       MSUB.100
 1106 IR   = I                                                          MSUB.101
      TY =  ABS  ( Y(I) )                                               MSUB.102
 1104   CONTINUE                                                        MSUB.103
C                       TEST PIVOT                                      MSUB.104
      IF  (TY - TPIV )    1107, 1108, 1108                              MSUB.105
C        BAD  PIVOT,  ROW IR,  COLUMN JT                                MSUB.106
 1107 KB(JT)= 0                                                         MSUB.107
      GO TO 1102                                                        MSUB.108
C                       PIVOT                                           MSUB.109
 1108 JH(IR) = JT                                                       MSUB.110
      KB(JT) = IR                                                       MSUB.111
      GO TO 900                                                         MSUB.112
C 900 CALL PIV    (IR, Y, M, E, Z, X)                                   MSUB.113
 1102     CONTINUE                                                      MSUB.114
C                 RESET ARTIFICIALS                                    MSUB.115
        DO 1109  I = 1, M                                               MSUB.116
      IF ( JH(I) - 12345  )  1109, 1112, 1109                           MSUB.117
 1112 JH(I) = 0                                                         MSUB.118
 1109  CONTINUE                                                        MSUB.119
C**END OF VER                                                           MSUB.120
C                                                                       MSUB.121
C                                                                       MSUB.122
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  100 ASSIGN   705  TO  NDEL                                          MSUB.123
      ASSIGN  1000  TO  KJMY                                          MSUB.124
      ASSIGN   221  TO  KPIV                                          MSUB.125
C                                                                     MSUB.126
C                              PERFORM ONE ITERATION                  MSUB.127
C                                                                     MSUB.128
C  XCK 1    X CHECKER                                                 MSUB.129
C*****SUBROUTINE XCK ( M, MF, JH, X, TZERO, JIN )                     MSUB.130
C                                                                     MSUB.131
C           RESET X AND CHECK FOR INFEASIBILITIES                     MSUB.132
 1200   JIN  =  0                                                     MSUB.133
      NEG = 0                                                         MSUB.134
      DO 1201 I = MF, M                                               MSUB.135
      IF ( ABS  ( X(I) )  - TZERO)  1202, 1203, 1203                  MSUB.136
 1202 X(I) = 0.0                                                      MSUB.137
      GO TO 1201                                                      MSUB.138
 1203 IF ( X(I) )  1208, 1201, 1205                                   MSUB.139
 1205 IF ( JH(I) )  1201, 1206, 1201                                  MSUB.140
 1208 NEG = 1                                                         MSUB.141
 1206   JIN = 1                                                       MSUB.142
 1201   CONTINUE                                                      MSUB.143
C**END OF XCK                                                         MSUB.144
C                                                                     MSUB.145
C                                                                     MSUB.146
C           CHECK CHANGE OF PHASE.. GO BACK TO INVERT IF GONE INFEAS. MSUB.147
      IF (INFS - JIN ) 1320,  500,  200                               MSUB.148
C                  BECOME FEASIBLE                                    MSUB.149
  200 INFS = 0                                                        MSUB.150
  201 PMIX  =  0.0                                                    MSUB.151
C                                                                     MSUB.152
C  GET 1    GET PRICES                                               MSUB.153
C*****SUBROUTINE GET ( M, MC, MF, JH, X, P, E, INFS, PMIX )          MSUB.154
C                                                                     MSUB.155
  500 MM  = MC                                                        MSUB.156
C                          PRIMAL PRICES                              MSUB.157
  502 DO 503 J = 1, M                                                 MSUB.158
      P(J) = E(MM )                                                   MSUB.159
  503 MM  =MM  + M                                                    MSUB.160
      IF ( INFS )  501, 599, 501                                      MSUB.161
C                          COMPOSITE PRICES                           MSUB.162
  501 DO 504  J = 1, M                                                MSUB.163
  504 P(J) = P(J)* PMIX                                               MSUB.164
      DO 505  I = MF, M                                               MSUB.165
      MM  =I                                                          MSUB.166
      IF  ( X(I) )  506, 507, 507                                     MSUB.167
  506 DO 508  J = 1, M                                                MSUB.168
      P(J) =  P(J) + E(MM )                                           MSUB.169
  508 MM  = MM  + M                                                   MSUB.170
      GO TO 505                                                       MSUB.171
  507 IF (JH(I))  505, 509, 505                                       MSUB.172
  509 DO 510  J = 1, M                                                MSUB.173
      P(J) = P(J) - E(MM )                                            MSUB.174
  510 MM  =  MM  +M                                                   MSUB.175
  505   CONTINUE                                                      MSUB.176
C                                                                     MSUB.177
  599 CONTINUE                                                        MSUB.178
C**END OF GET                                                         MSUB.179
C                                                                     MSUB.180
C                                                                     MSUB.181
C                                                                     MSUB.182
C    MIN          MIN D-J.  SELECTS COLUMN TO ENIER BASIS             MSUB.183
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C*****SUBROUTINE MIN ( JT, N, M, A, P, KB, ME, TCOST )                  MSUB.184
C                                                                       MSUB.185
  700 JT = 0                                                            MSUB.186
      BB = TCOST                                                        MSUB.187
C                                                                       MSUB.188
  701 DO  702  JM = 1, N                                                MSUB.189
C                                  SKIP COLUMNS IN BASIS                MSUB.190
  703 IF ( KB(JM) )  702, 300, 702                                      MSUB.191
C 300 CALL DEL ( JM, DT, M, A, P)                                       MSUB.192
  705 IF  ( DT - BB )  708, 702, 702                                    MSUB.193
  708 BB = DT                                                           MSUB.194
      JT = JM                                                           MSUB.195
  702    CONTINUE                                                       MSUB.196
C                                                                       MSUB.197
C**END OF MIN                                                           MSUB.198
C                                                                       MSUB.199
       IF  (JT)    203, 203, 600                                        MSUB.200
C           ALL COSTS NON-NEGATIVE...  K = 3 OR 4                       MSUB.201
  203 K = 3 + INFS                                                      MSUB.202
      GO TO 257                                                         MSUB.203
C                                  NORMAL CYCLE                         MSUB.204
C                                                                       MSUB.205
C  JMY 1          J MULTIPLY.  BASIS INVERSE * COLUMN JT                MSUB.206
C*****SUBROUTINE JMY (JT, A, E, M, Y, ME )                              MSUB.207
C                                                                       MSUB.208
  600 DO 610  I= 1,M                                                    MSUB.209
  610 Y(I) =0.                                                          MSUB.210
      LP  =  JT*ME - ME                                                 MSUB.211
      LL = 0                                                            MSUB.212
      DO 605   I= 1,M                                                   MSUB.213
      LP = LP + 1                                                       MSUB.214
      IF  (A(LP))   601, 602, 601                                       MSUB.215
  601 DO 606  J  =  1,M                                                 MSUB.216
      LL = LL + 1                                                       MSUB.217
  606 Y(J) = Y(J) + A(LP) * E(LL)                                       MSUB.218
      GO TO 605                                                         MSUB.219
  602 LL = LL + M                                                       MSUB.220
  605 CONTINUE                                                          MSUB.221
C                                                                       MSUB.222
  699 GO TO KJMY , ( 1000 , 1114 ,  1392  )                             MSUB.223
C**END OF JMY                                                           MSUB.224
C                                                                       MSUB.225
C                                                                       MSUB.226
C  ROW 1    ROW SELECTION--COMPOSITE                                    MSUB.227
C*****SUBROUTINE  ROW  ( IR, M, MF, JH, X, Y, IPIV )                    MSUB.228
C                                                                       MSUB.229
C AMONG EQS. WITH X=0, FIND MAX ABS(Y) AMONG ARTIFICIALS, OR, IF NONE,  MSUB.230
C  GET MAX POSITIVE Y(I) AMONG REALS.                                   MSUB.231
 1000 IR = 0                                                            MSUB.232
      AA = 0.0                                                          MSUB.233
      IA  =  0                                                          MSUB.234
      DO 1050  I = MF,  M                                               MSUB.235
      IF ( X(I) )  1050, 1041, 1050                                     MSUB.236
 1041 YI  =  ABS  ( Y(I) )                                              MSUB.237
      IF  (  YI  -  TPIV   )   1050, 1050, 1042                         MSUB.238
 1042 IF  ( JH(I) )  1043, 1044, 1043                                   MSUB.239
 1043 IF  (IA)   1050, 1048, 1050                                       MSUB.240
 1048  IF  ( Y(I) )  1050, 1050, 1045                                   MSUB.241
 1044 IF   (IA)   1045, 1046, 1045                                      MSUB.242
 1045 IF   (  YI    -  AA   )   1050, 1050, 1047                        MSUB.243
 1046    IA = 1                                                         MSUB.244
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 1047 AA  =  YI                                                          MSUB.245
      IR  =  I                                                           MSUB.246
 1050 CONTINUE                                                           MSUB.247
      IF (IR)1099,1001,1099                                              MSUB.248
 1001 AA = 1.0E+20                                                       MSUB.249
C                FIND MIN. PIVOT AMONG POSITIVE EQUATIONS               MSUB.250
      DO 1010 IT = MF , M                                                MSUB.251
      IF  ( Y(IT)  -  TPIV )  1010, 1010, 1002                           MSUB.252
 1002 IF  ( X(IT) ) 1010, 1010, 1003                                     MSUB.253
 1003 XY = X(IT) / Y(IT)                                                 MSUB.254
      IF ( XY - AA )  1004, 1005, 1010                                   MSUB.255
 1005 IF ( JH(IT))  1010, 1004, 1010                                     MSUB.256
 1004 AA = XY                                                            MSUB.257
      IR = IT                                                            MSUB.258
 1010 CONTINUE                                                           MSUB.259
      IF (NEG)   1016, 1099, 1016                                        MSUB.260
C  FIND PIVOT AMONG NEGATIVE EQUATIONS, IN WHICH X/Y IS LESS THAN THE     MSUB.261
C MINIMUM X/Y IN THE POSITIVE EQUATIONS, THAT HAS THE LARGEST ABSF(Y)     MSUB.262
 1016 BB = - TPIV                                                        MSUB.263
      DO 1030 I  = MF , M                                                MSUB.264
      IF (X(I))   1012, 1030, 1030                                       MSUB.265
 1012  IF  ( Y(I)    -  BB  )   1022, 1030, 1030                         MSUB.266
 1022 IF  (  Y(I) * AA  -  X(I)   )   1024, 1024, 1030                   MSUB.267
 1024 BB  =  Y(I)                                                        MSUB.268
      IR  =  I                                                           MSUB.269
 1030 CONTINUE                                                           MSUB.270
 1099 CONTINUE                                                           MSUB.271
C**END OF ROW                                                            MSUB.272
C                                                                        MSUB.273
C                              TEST PIVOT                                MSUB.274
  206   IF( IR )   207, 207, 210                                         MSUB.275
C                              NO PIVOT                                  MSUB.276
  207 K = 5                                                              MSUB.277
  257 IF (PMIX)   201, 400, 201                                          MSUB.278
C                         ITERATION LIMIT FOR CUT OFF                    MSUB.279
  210 IF (ITER -NCUT )    900,  160,  160                                MSUB.280
C                              PIVOT FOUND                               MSUB.281
C                                                                        MSUB.282
C  PIV 1          PIVOT.  PIVOTS ON GIVEN ROW                            MSUB.283
C*****SUBROUTINE PIV  ( IR, Y, M, E, X, NUMPV, TECOL )                   MSUB.284
C                         LEAVE TRANSFORMED COLUMN IN Y(I)               MSUB.285
C                                                                        MSUB.286
  900 NUMPV  =  NUMPV  +  1                                              MSUB.287
      YI = -Y(IR)                                                        MSUB.288
      Y(IR) = -1.                                                        MSUB.289
      LL = 0                                                             MSUB.290
C                              TRANSFORM INVERSE                         MSUB.291
  903 DO 904  L =  IR, M2, M                                             MSUB.292
      IF  ( E(L) )  905, 914, 905                                        MSUB.293
  914 LL = LL + M                                                        MSUB.294
      GO TO 904                                                          MSUB.295
  905 XY =  E(L) / YI                                                    MSUB.296
      E(L) =0.                                                           MSUB.297
      DO 906  I  = 1, M                                                  MSUB.298
      LL= LL +1                                                          MSUB.299
  906 E(LL) = E(LL) +XY* Y(I)                                            MSUB.300
  904 CONTINUE                                                           MSUB.301
C                              TRANSFORM X                               MSUB.302
       XY = X(IR) / YI                                                   MSUB.303
      X(IR) = 0.                                                         MSUB.304
      DO 908  I  = 1, M                                                  MSUB.305
```

```
  908 X(I) = X(I) +XY* Y(I)                                              MSUB.306
C                          RESTORE Y(IR)                                 MSUB.307
      Y(IR) = -YI                                                        MSUB.308
C                                                                        MSUB.309
  999  GO TO KPIV , ( 221, 1102 )                                        MSUB.310
C**END OF PIV                                                            MSUB.311
C                                                                        MSUB.312
  221  IA    = JH(IR)                                                    MSUB.313
      IF ( IA ) 213, 213, 214                                            MSUB.314
  214 KB( IA ) = 0                                                       MSUB.315
  213 KB(JT)   = IR                                                      MSUB.316
      JH(IR)   = JT                                                      MSUB.317
      LA   =  0                                                          MSUB.318
      ITER    = ITER    +1                                               MSUB.319
      INVC    = INVC    +1                                               MSUB.320
C                           INVERSION FREQUENCY                          MSUB.321
      IF (INVC - NVER  ) 1200, 1320,1200                                 MSUB.322
C                                      CUT OFF ... TOO MANY ITERATIONS   MSUB.323
  160 K = 6                                                              MSUB.324
C                                                                        MSUB.325
C                                                                        MSUB.326
C  ERR 1          ERROR CHECK.  COMPARES AX WITH B, PA WITH ZERO         MSUB.327
C*****SUBROUTINE ERR ( M, A, B, TERR, JH, X, P, Y, ME, LA )              MSUB.328
C                                                                        MSUB.329
C                                  STORE AX-B AT Y                       MSUB.330
  400  ASSIGN 410 TO NDEL                                                MSUB.331
      DO 401 I = 1, M                                                    MSUB.332
  401 Y(I) =-B(I)                                                        MSUB.333
      DO 402 I = 1, M                                                    MSUB.334
      JA = JH(I)                                                         MSUB.335
      IF (JA) 403, 402, 403                                              MSUB.336
  403 IA =ME* (JA-1)                                                     MSUB.337
      DO 405 IT = 1, M                                                   MSUB.338
      IA = IA + 1                                                        MSUB.339
      IF(A(IA) )  415, 405, 415                                          MSUB.340
  415 Y(IT) =Y(IT) +X(I) * A(IA)                                         MSUB.341
  405 CONTINUE                                                           MSUB.342
  402 CONTINUE                                                           MSUB.343
C                                  FIND SUM AND MAXIMUM OF ERRORS        MSUB.344
      DO 481  I = 1, M                                                   MSUB.345
      YI   = Y(I)                                                        MSUB.346
      IF ( JH(I) )  472, 471, 472                                        MSUB.347
  471  YI = YI + X(I)                                                    MSUB.348
  472 TERR(LA+1) = TERR(LA+1) + ABS (YI)                                 MSUB.349
      IF  ( ABS  (TERR(LA+2))- ABS  (  YI  )  )   482, 481, 481          MSUB.350
  482 TERR(LA+2) = YI                                                    MSUB.351
  481   CONTINUE                                                         MSUB.352
C                                  STORE P TIMES BASIS AT DT             MSUB.353
      DO 411  I = 1, M                                                   MSUB.354
      JM = JH(I)                                                         MSUB.355
      IF ( JM    )  300 , 411 , 300                                      MSUB.356
C 300 CALL DEL ( JM, DT, M, A, P)                                        MSUB.357
  410 TERR(LA+3)  =  TERR(LA +3)  +  ABS (DT)                            MSUB.358
      IF (ABS (TERR(LA+4))   -   ABS (DT)  )  413, 411, 411              MSUB.359
  413  TERR(LA+4)  =  DT                                                 MSUB.360
  411 CONTINUE                                                           MSUB.361
C**END OF ERR                                                            MSUB.362
C                                                                        MSUB.363
C                                                                        MSUB.364
      IF (LA)   193, 191,  193                                           MSUB.365
  191 LA  =  4                                                           MSUB.366
```

```
      IF (INFLAG  -  4  )  1320,  193,  193                              MSUB.367
  193 IF  (K-5)    1392,  194,  1392                                     MSUB.368
  194 ASSIGN 1392 TO KJMY                                                MSUB.369
      GO TO 600                                                          MSUB.370
C 600 CALL JMY ( . . . . . )                                             MSUB.371
C     GO TO 1392                                                         MSUB.372
 1304 K  =  7                                                            MSUB.373
C                 SET EXIT VALUES                                        MSUB.374
 1392   DO  1309  I=  1, 8                                              MSUB.375
 1309 ERR(I)          =   TERR(I)                                        MSUB.376
      DO 1329  I = 1, 7                                                  MSUB.377
 1329 KOUT(I)  =  IOFIX(I+8)                                             MSUB.378
      RETURN                                                             MSUB.379
C                                                                        MSUB.380
C    DEL          DELTA-JAY.  PRICES OUT ONE MATRIX COLUMN              MSUB.381
C*****SUBROUTINE DEL (  JM, DT, M, A, P, ME )                            MSUB.382
C                                                                        MSUB.383
C                                                                        MSUB.384
  300 DT = 0.                                                            MSUB.385
      LL  = (JM - 1) * ME                                                MSUB.386
  301 DO  303   MM  = 1, M                                               MSUB.387
      LL   =  LL  + 1                                                    MSUB.388
      IF ( A( LL ))304, 303, 304                                         MSUB.389
  304 DT = DT + P( MM ) * A ( LL )                                       MSUB.390
  303 CONTINUE                                                           MSUB.391
C                                                                        MSUB.392
  399   GO TO NDEL , ( 410 , 705 )                                       MSUB.393
C**END OF DEL                                                            MSUB.394
C                                                                        MSUB.395
      END                                                                MSUB.396
```

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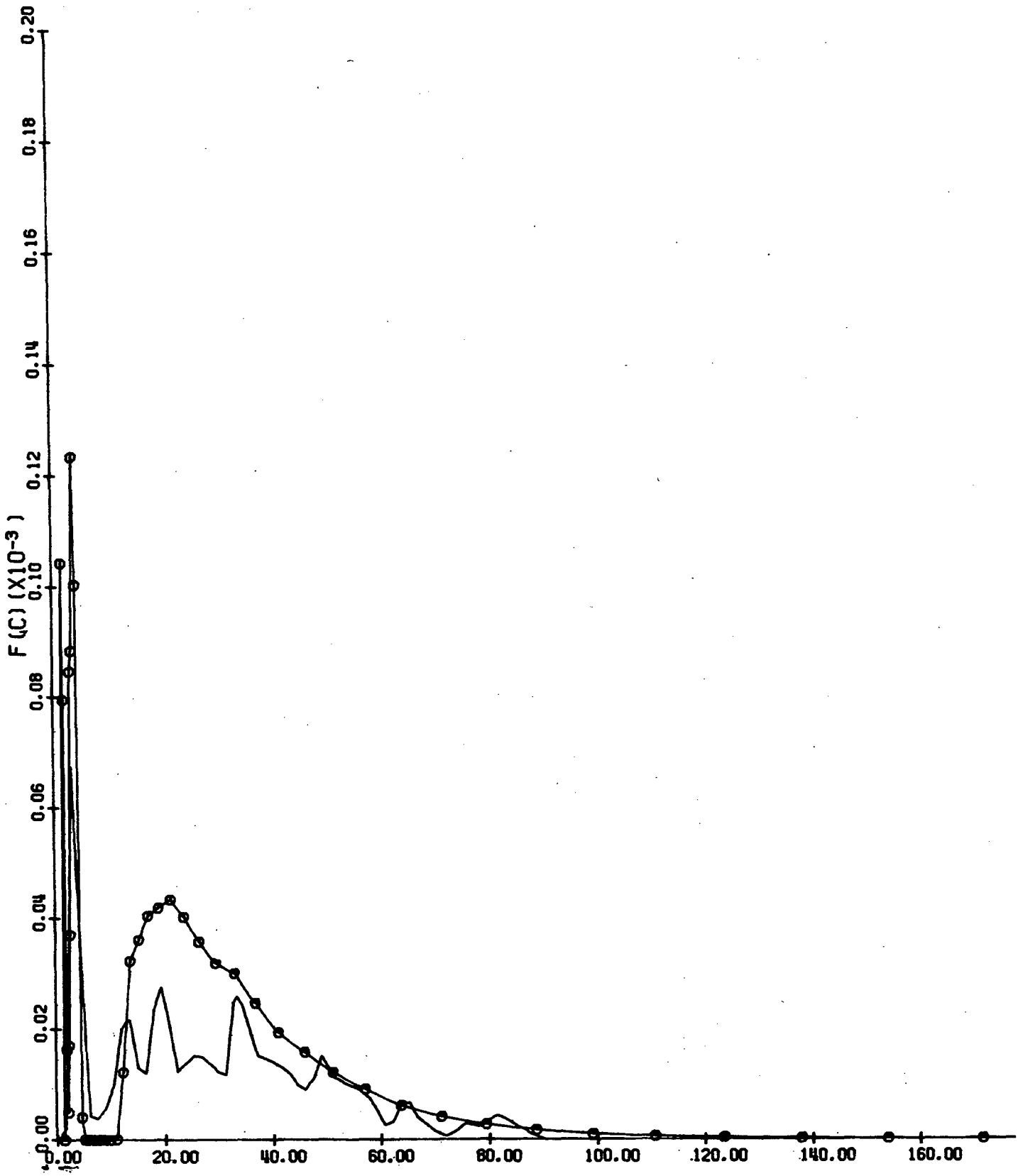
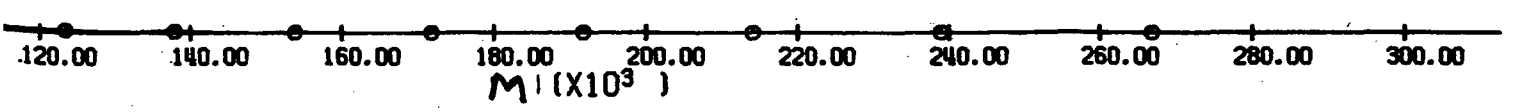


Figure 1. Resulting MWD Using Ten Sets of Molecular Weights a



Ten Sets of Molecular Weights and g = 3.0, (Compare with Figures 2-4)

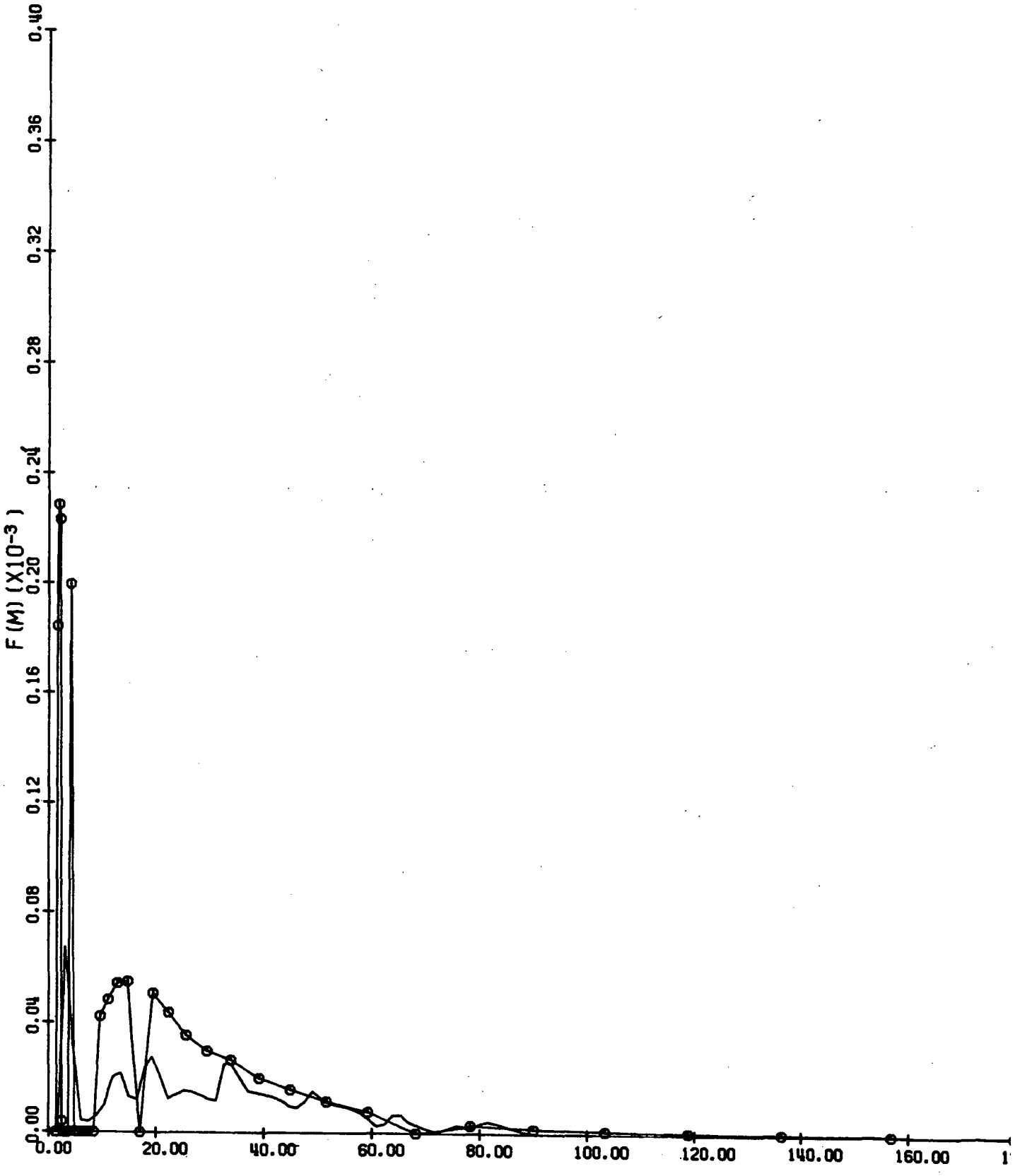
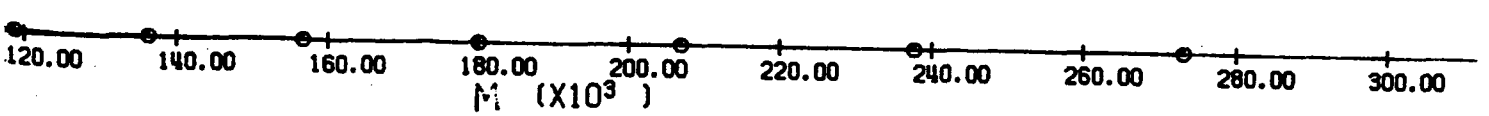


Figure 2. Resulting MWD Using Ten Sets of Molecular Weights and g =



Sets of Molecular Weights and g = 4.0, (Compare with Figures 1, 3, and 4)

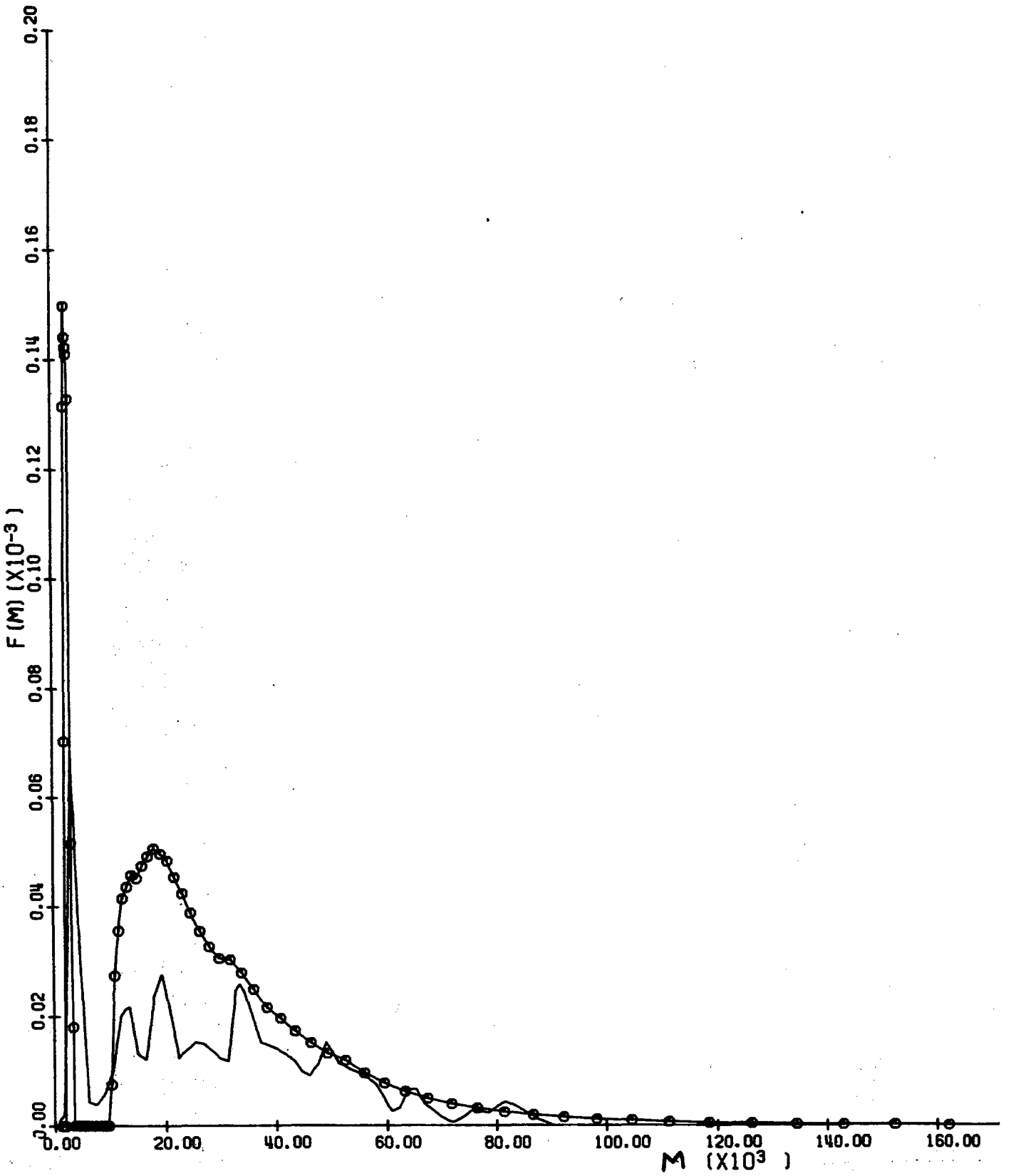
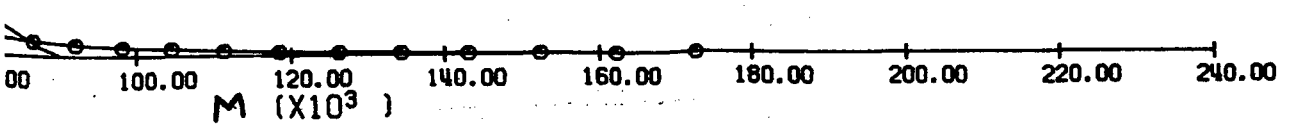


Figure 3. Resulting MWD Using Twenty Sets of Molecular Weights and g = 3.5, (Co



enty Sets of Molecular Weights and g = 3.5, (Compare with Figures 1, 2, and 4)

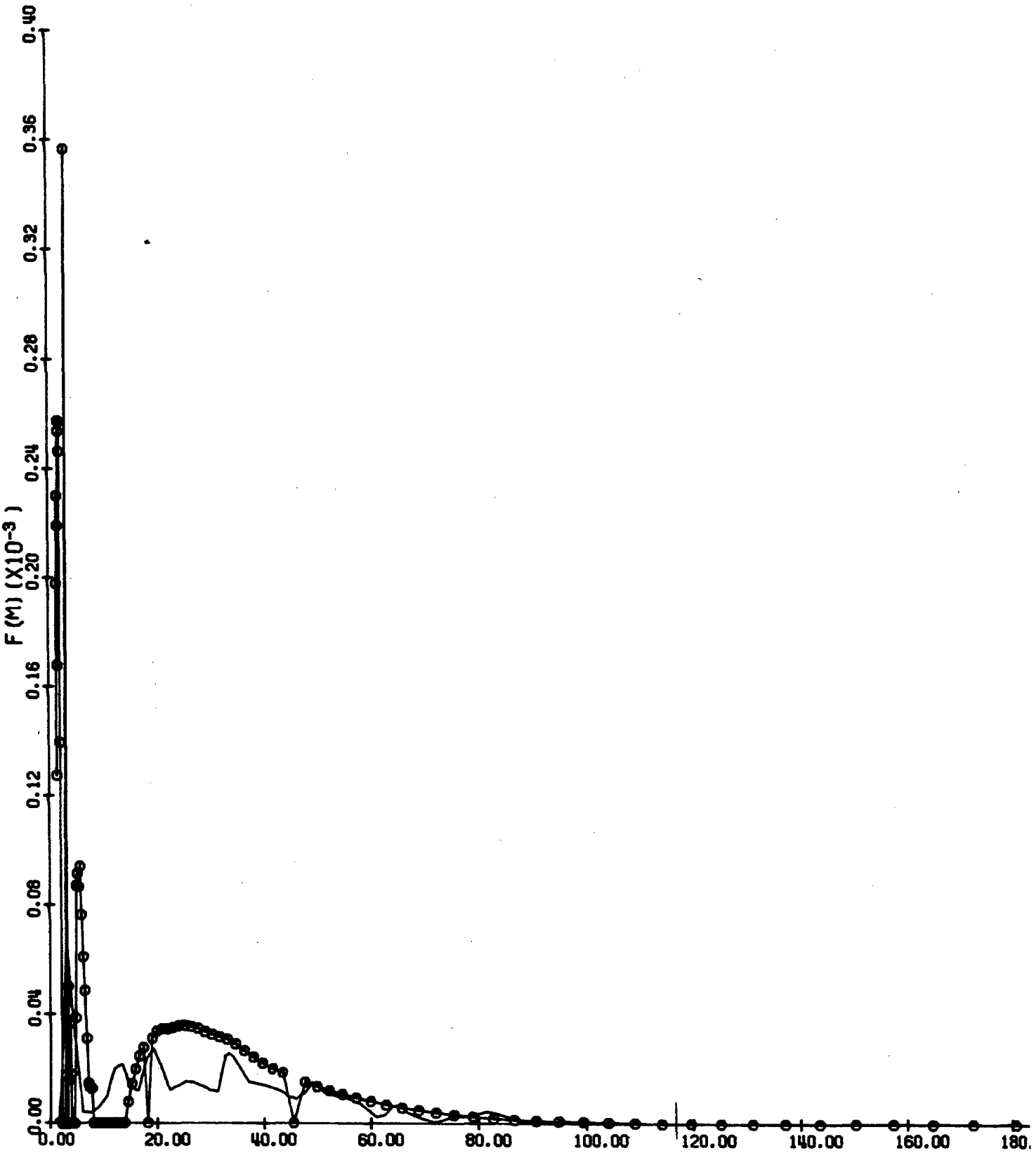
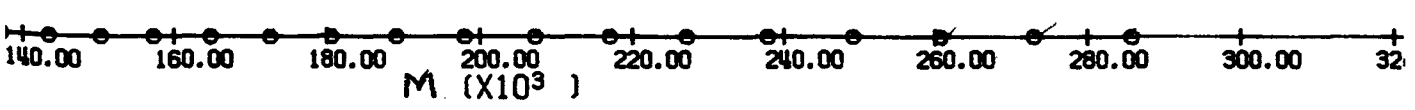


Figure 4. Resulting MWD Using Twenty Sets of Molecular W



enty Sets of Molecular Weights and g = 2.5, (Compare with Figures 1-3)

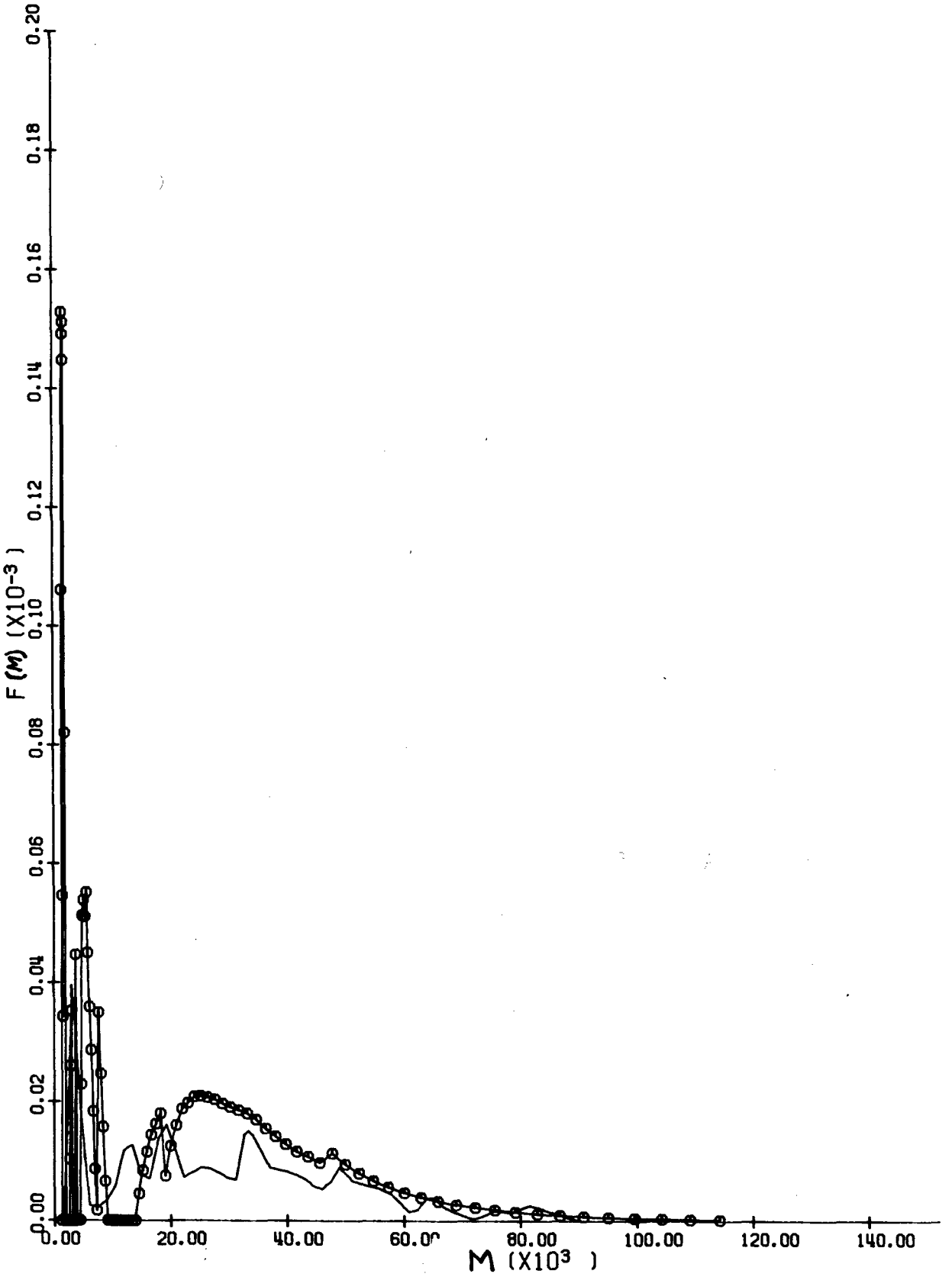


Figure 5. The Effect of Decreasing the MWR on the MWD

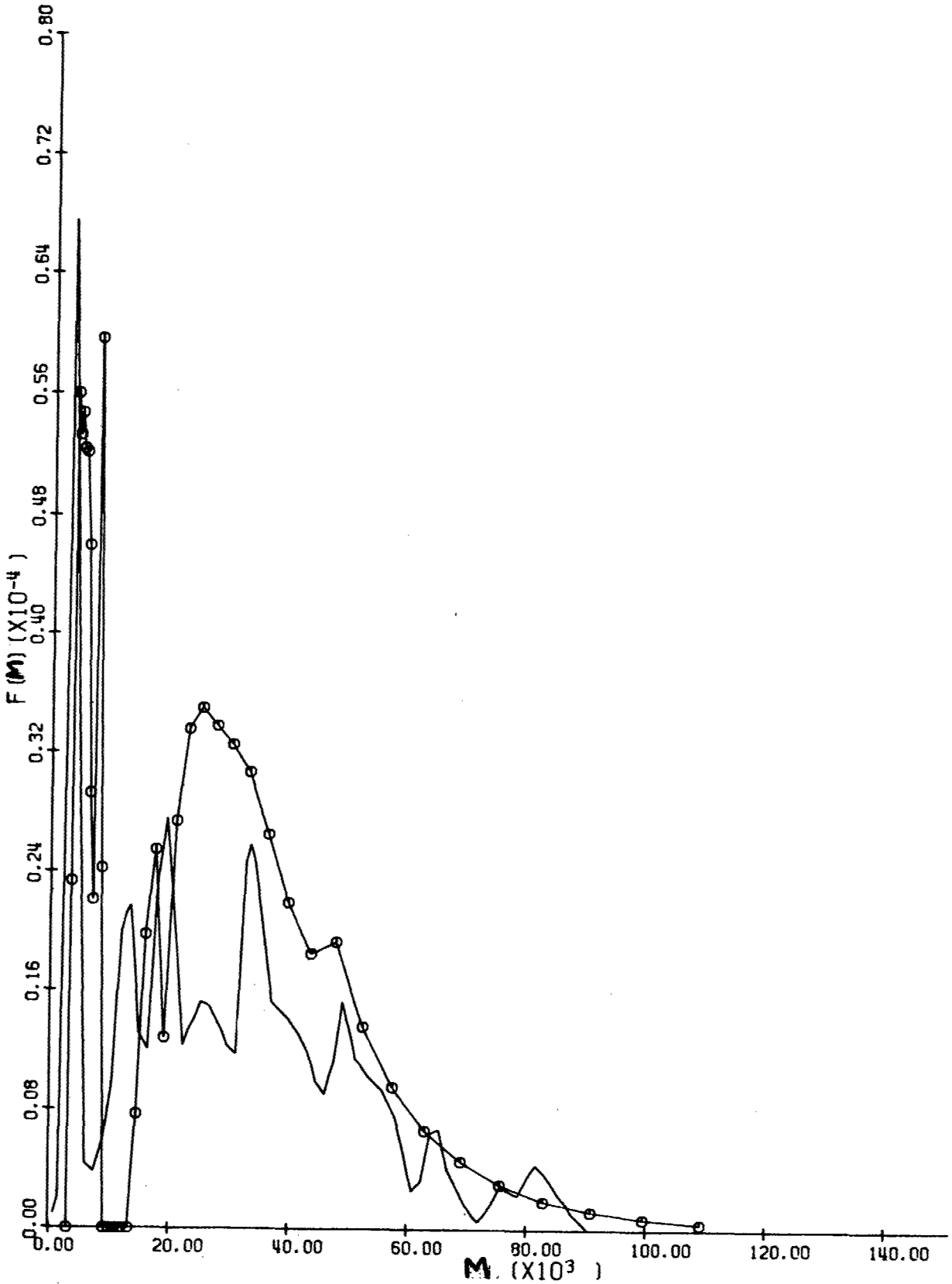


Figure 6. The Effect of Decreasing the MWR and the Number of Molecular Weight Sets on the MWD

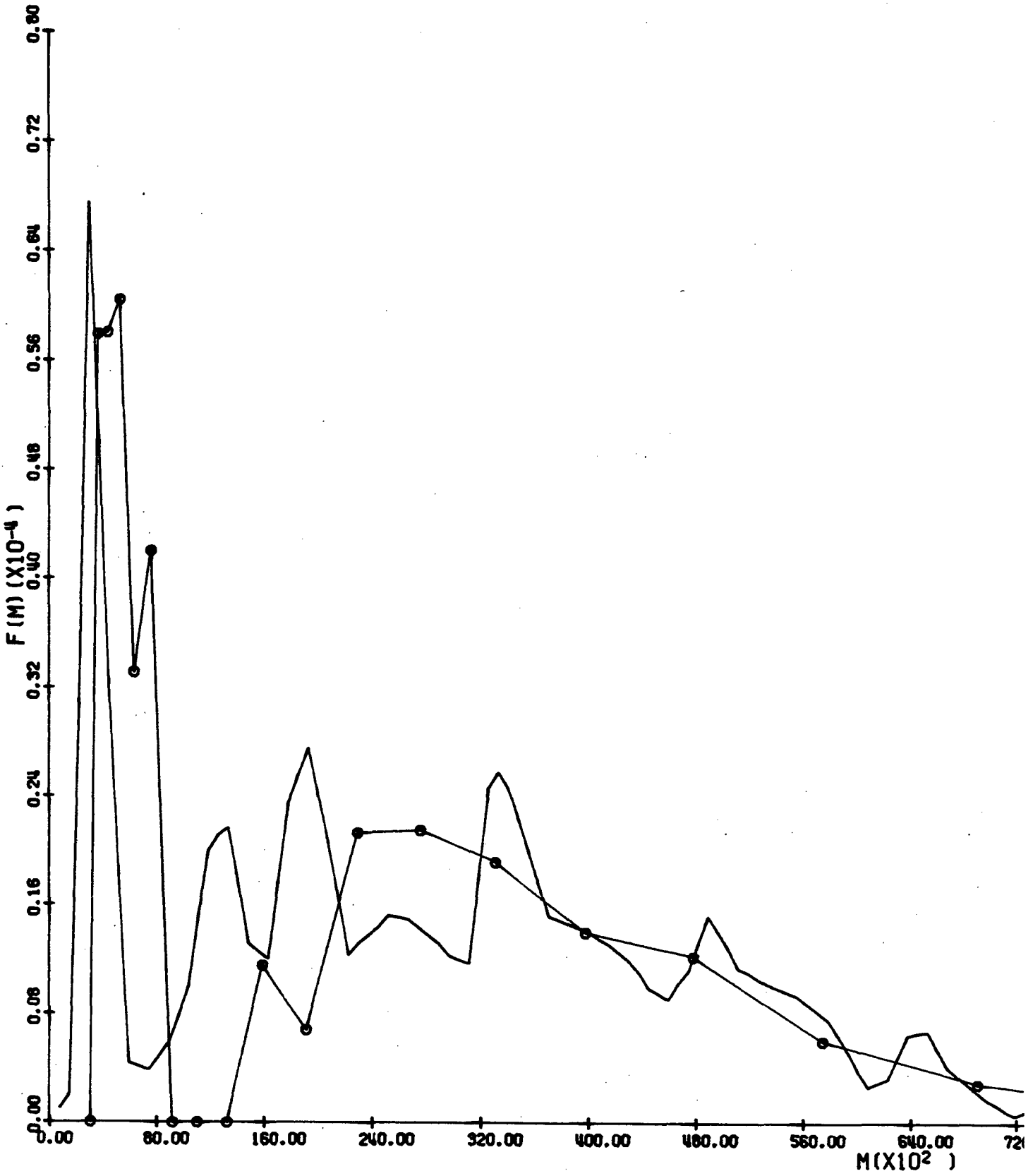
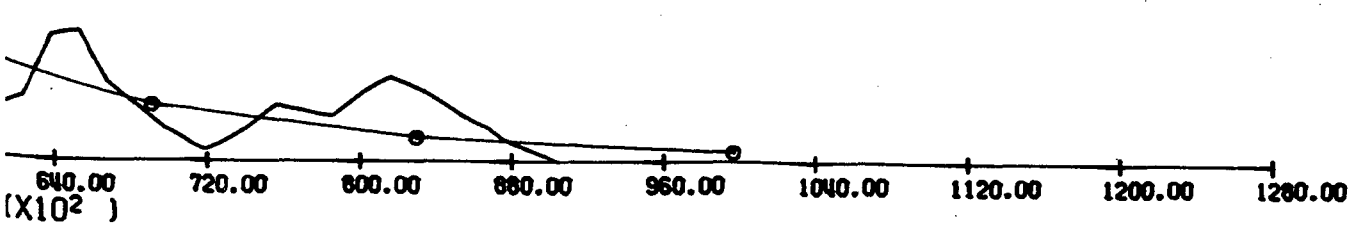


Figure 7. The Effect of Further Decreasing t



er Decreasing the Number of Molecular Weight Sets

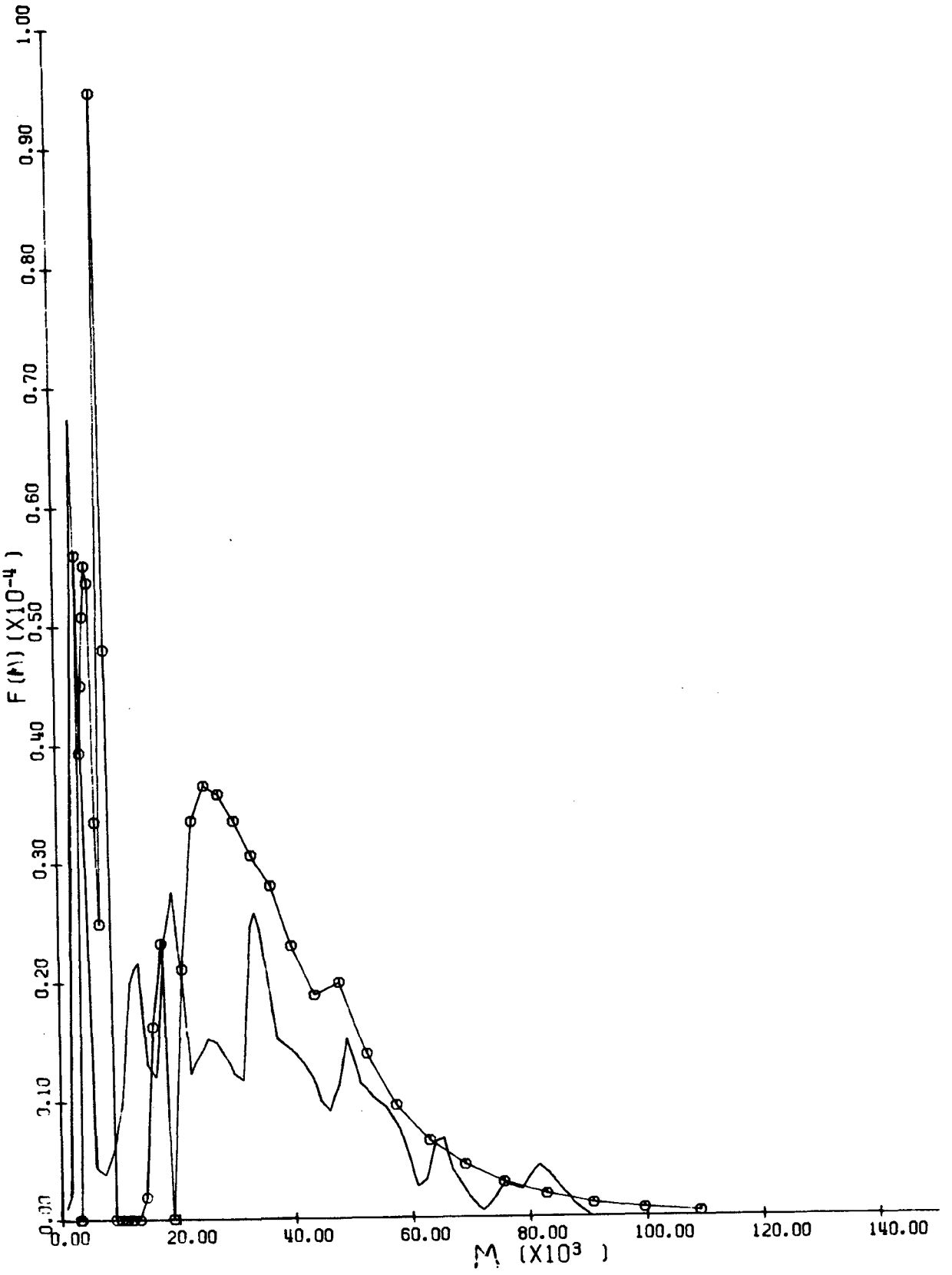


Figure 8. The Effect of Using More Experimental Data on the MWD

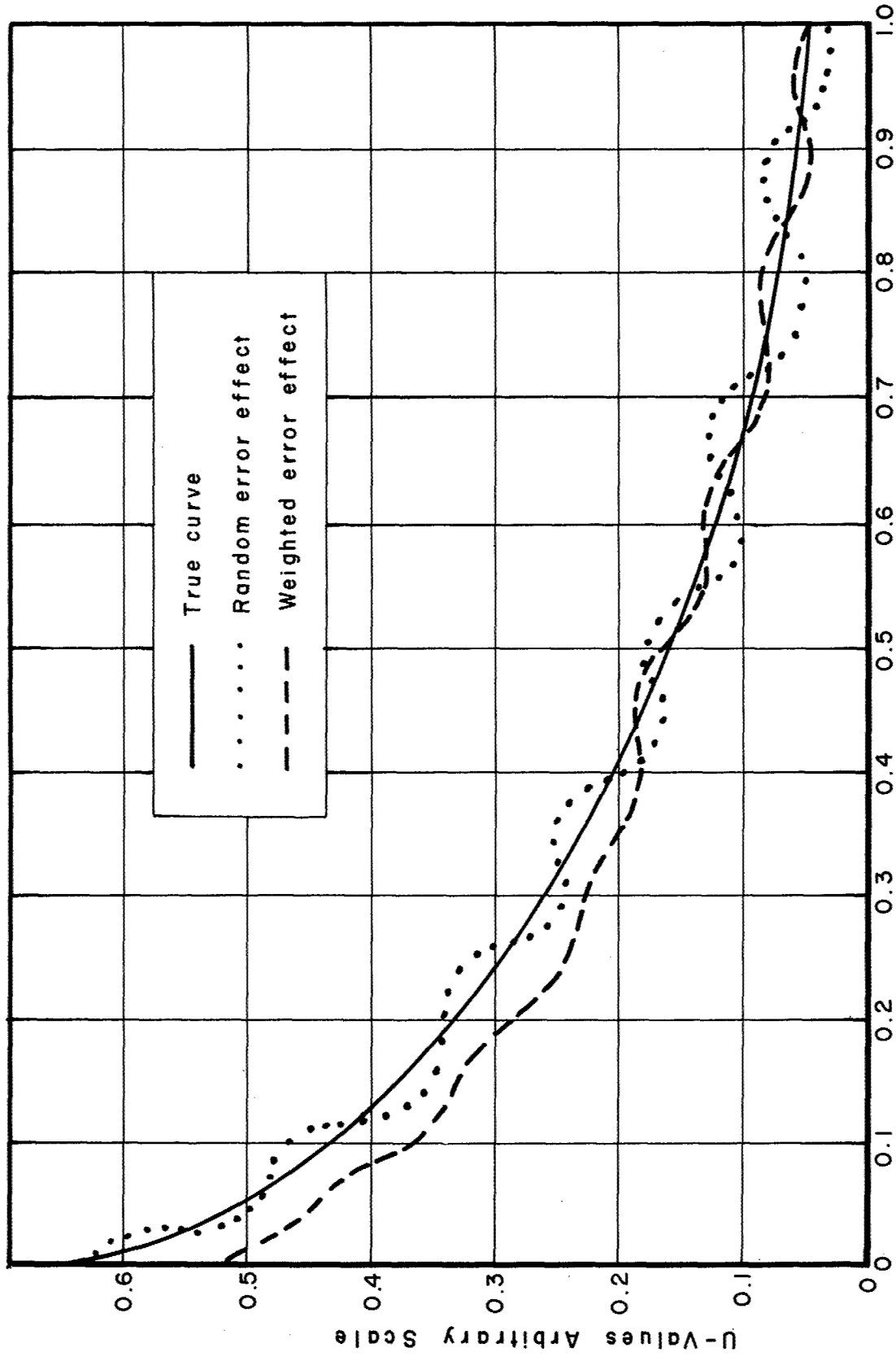


Figure 9. A Typical Curve of Concentration Gradient from One Angular Velocity

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13. ABSTRACT

Within the past decade easy access to high speed digital computers has renewed interest in deriving a molecular weight distribution from equilibrium sedimentation-diffusion data. One of the computational schemes which appears most promising is the Simplex Method of linear programming. The purpose of this work was to investigate the advantages and limitations of this approach.

It was found that even though inferring a molecular weight distribution from equilibrium sedimentation-diffusion data is mathematically an ill-posed problem, the method of linear programming yields qualitatively a good molecular weight distribution. Also, the method is applicable to the case of one angular velocity.

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Polydispersity						
Linear Programming						
Molecular Weight Distribution						
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